Full wwPDB EM Validation Report

Apr 8, 2024 – 11:50 AM EDT

PDB ID	:	8TPJ
EMDB ID	:	EMD-41475
Title	:	Top cylinder bound to OCP from high-resolution phycobilisome quenched by OCP (local refinement)
Authors	:	Sauer, P.V.; Sutter, M.; Cupellini, L.
Deposited on	:	2023-08-04
Resolution	:	2.10 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

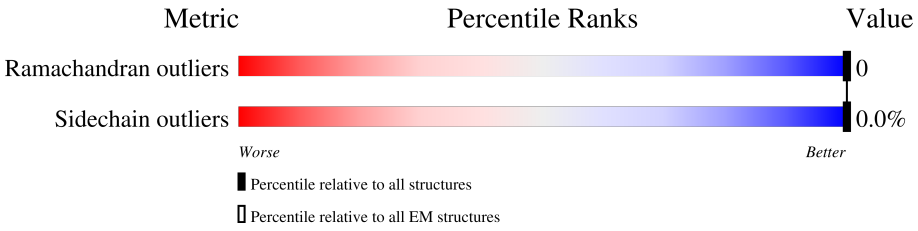
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	896	23% 77%
2	B	317	46% 93% 7%
2	b	317	38% 41% 59%
3	C	67	100%
4	D	161	99%
4	F	161	99%
4	H	161	99%
4	J	161	99%
4	L	161	99%

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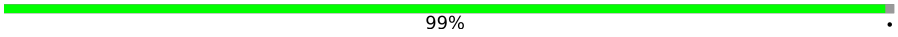
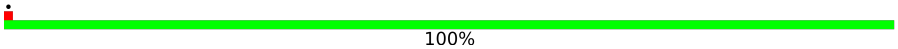
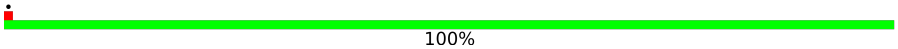
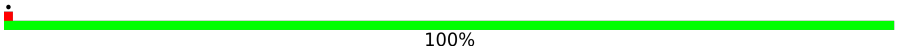
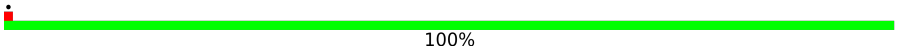
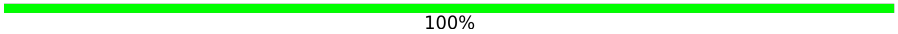
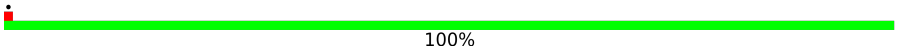
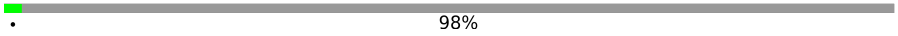
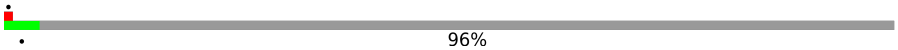
Mol	Chain	Length	Quality of chain
4	N	161	
5	E	161	
5	G	161	
5	I	161	
5	K	161	
5	M	161	
5	O	161	
6	P	249	
6	Q	249	
6	R	249	
6	S	249	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 45170 atoms, of which 21441 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Phycobiliprotein ApcE.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	210	3396	1083	1704	289	316	4	0	0

- Molecule 2 is a protein called Orange carotenoid-binding protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	296	4567	1459	2287	387	423	11	0	0
			Total	C	H	N	O	S		
2	b	130	2050	659	1025	172	191	3	0	0

- Molecule 3 is a protein called Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	67	1114	343	568	104	94	5	0	0

- Molecule 4 is a protein called Allophycocyanin alpha chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	D	160	2420	754	1210	207	242	7	0	0
			Total	C	H	N	O	S		
4	F	160	2420	754	1210	207	242	7	0	0
			Total	C	H	N	O	S		
4	H	160	2420	754	1210	207	242	7	0	0
			Total	C	H	N	O	S		
4	J	160	2420	754	1210	207	242	7	0	0
			Total	C	H	N	O	S		
4	L	160	2420	754	1210	207	242	7	0	0
			Total	C	H	N	O	S		
4	N	160	2420	754	1210	207	242	7	0	0

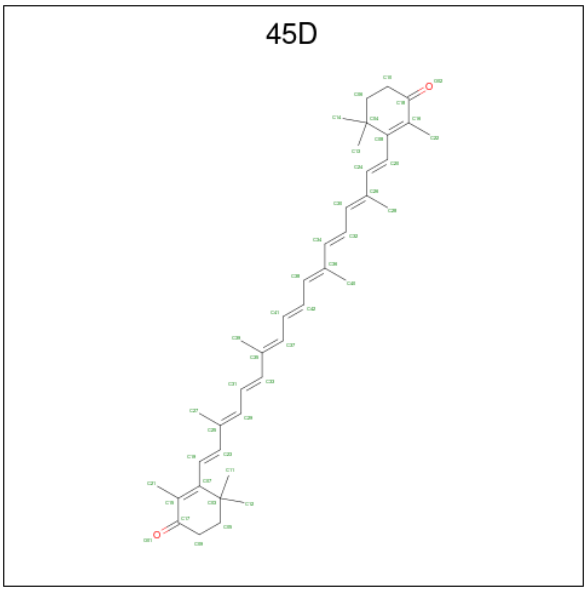
- Molecule 5 is a protein called Allophycocyanin beta chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	161	Total	C	H	N	O	S	0	0
			2427	758	1220	202	240	7		
5	G	161	Total	C	H	N	O	S	0	0
			2427	758	1220	202	240	7		
5	I	161	Total	C	H	N	O	S	0	0
			2427	758	1220	202	240	7		
5	K	161	Total	C	H	N	O	S	0	0
			2427	758	1220	202	240	7		
5	M	161	Total	C	H	N	O	S	0	0
			2427	758	1220	202	240	7		
5	O	161	Total	C	H	N	O	S	0	0
			2427	758	1220	202	240	7		

- Molecule 6 is a protein called Phycobilisome rod-core linker polypeptide CpcG.

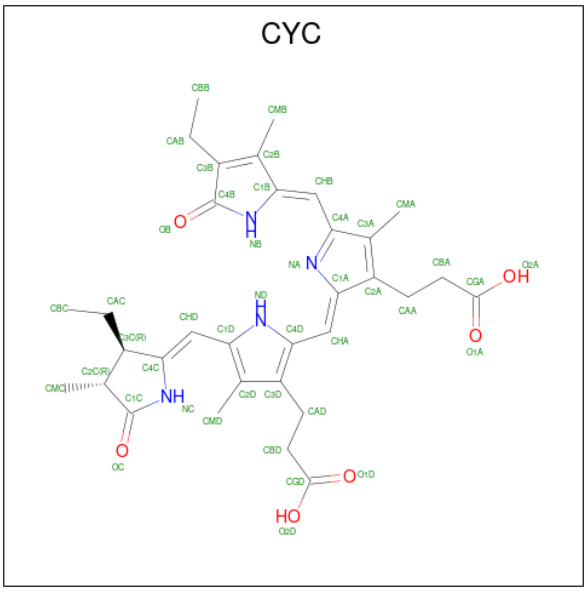
Mol	Chain	Residues	Atoms						AltConf	Trace
6	P	41	Total	C	H	N	O	S	0	0
			623	188	318	59	56	2		
6	Q	42	Total	C	H	N	O	S	0	0
			645	194	331	61	57	2		
6	R	4	Total	C	H	N	O		0	0
			86	27	45	10	4			
6	S	10	Total	C	H	N	O		0	0
			177	56	87	18	16			

- Molecule 7 is beta,beta-carotene-4,4'-dione (three-letter code: 45D) (formula: $C_{40}H_{52}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
7	B	1	Total	C	H	O	0
			94	40	52	2	

- Molecule 8 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: $C_{33}H_{40}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
8	D	1	Total	C	H	N	O	0
			80	33	37	4	6	
8	E	1	Total	C	H	N	O	0
			80	33	37	4	6	

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Mol	Chain	Residues	Atoms					AltConf
8	F	1	Total	C	H	N	O	0
			80	33	37	4	6	
8	G	1	Total	C	H	N	O	0
			80	33	37	4	6	
8	H	1	Total	C	H	N	O	0
			80	33	37	4	6	
8	I	1	Total	C	H	N	O	0
			80	33	37	4	6	
8	J	1	Total	C	H	N	O	0
			80	33	37	4	6	
8	K	1	Total	C	H	N	O	0
			80	33	37	4	6	
8	L	1	Total	C	H	N	O	0
			80	33	37	4	6	
8	M	1	Total	C	H	N	O	0
			80	33	37	4	6	
8	N	1	Total	C	H	N	O	0
			80	33	37	4	6	
8	O	1	Total	C	H	N	O	0
			80	33	37	4	6	

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		AltConf
9	A	231	Total	O	0
			231	231	
9	B	123	Total	O	0
			123	123	
9	b	3	Total	O	0
			3	3	
9	C	67	Total	O	0
			67	67	
9	D	112	Total	O	0
			112	112	
9	E	151	Total	O	0
			151	151	
9	F	120	Total	O	0
			120	120	
9	G	159	Total	O	0
			159	159	
9	H	171	Total	O	0
			171	171	

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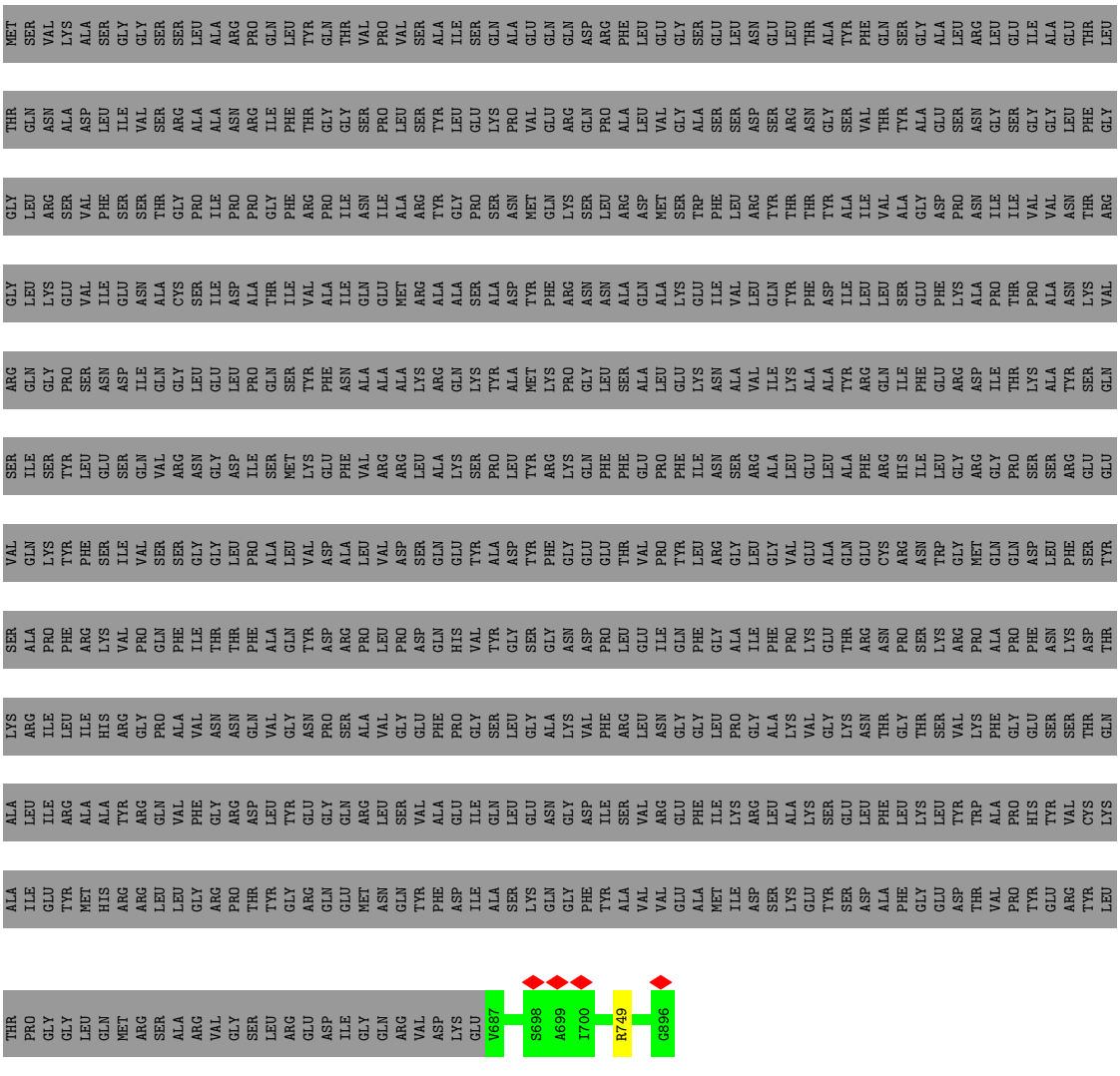
Mol	Chain	Residues	Atoms	AltConf
9	I	145	Total O 145 145	0
9	J	124	Total O 124 124	0
9	K	163	Total O 163 163	0
9	L	158	Total O 158 158	0
9	M	189	Total O 189 189	0
9	N	138	Total O 138 138	0
9	O	174	Total O 174 174	0
9	P	57	Total O 57 57	0
9	Q	61	Total O 61 61	0
9	R	15	Total O 15 15	0
9	S	15	Total O 15 15	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

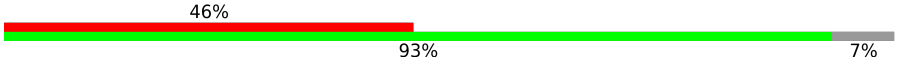
• Molecule 1: Phycobiliprotein ApcE

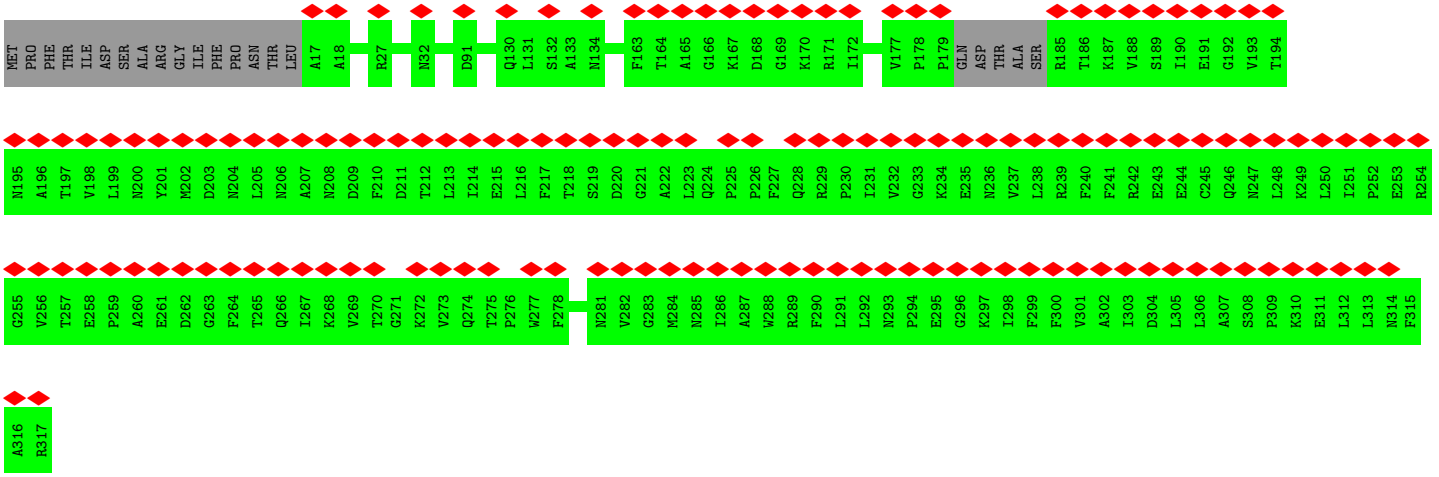
Chain A:



• Molecule 2: Orange carotenoid-binding protein

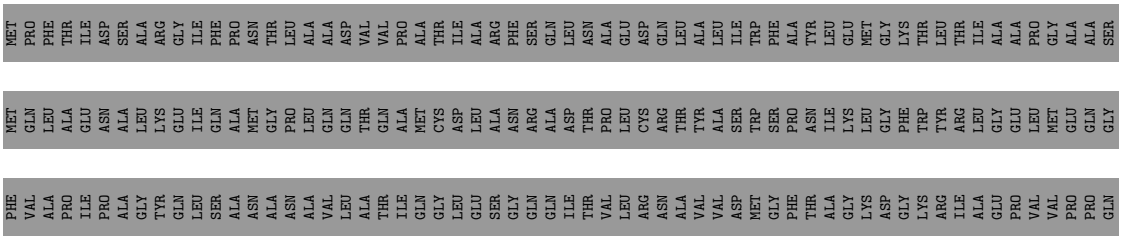
Chain B:

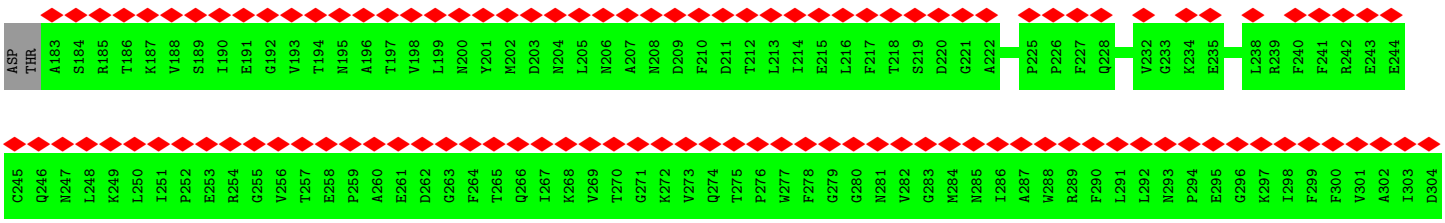




• Molecule 2: Orange carotenoid-binding protein

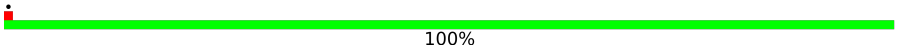
Chain b:





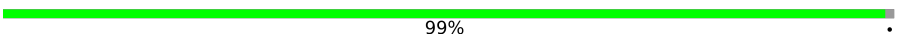
• Molecule 3: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain C:



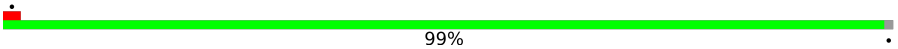
• Molecule 4: Allophycocyanin alpha chain

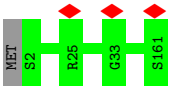
Chain D:



• Molecule 4: Allophycocyanin alpha chain

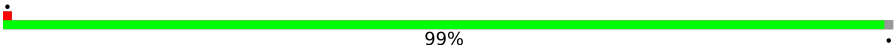
Chain F:

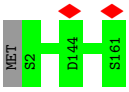




• Molecule 4: Allophycocyanin alpha chain

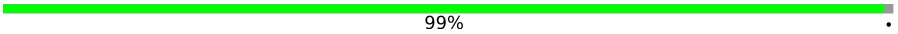
Chain H:





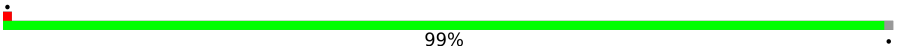
• Molecule 4: Allophycocyanin alpha chain

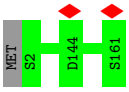
Chain J:



• Molecule 4: Allophycocyanin alpha chain

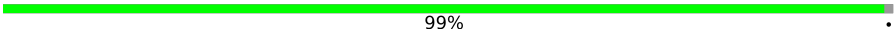
Chain L:





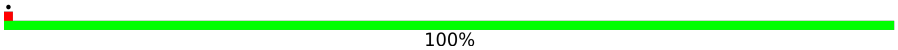
• Molecule 4: Allophycocyanin alpha chain

Chain N:



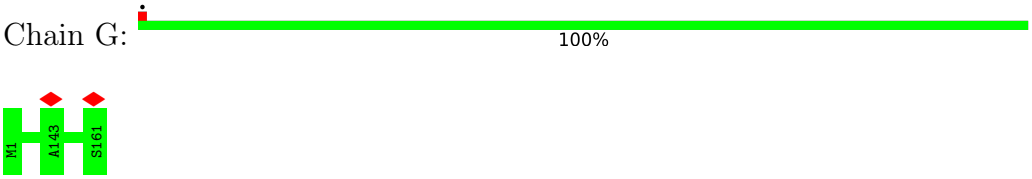
• Molecule 5: Allophycocyanin beta chain

Chain E:



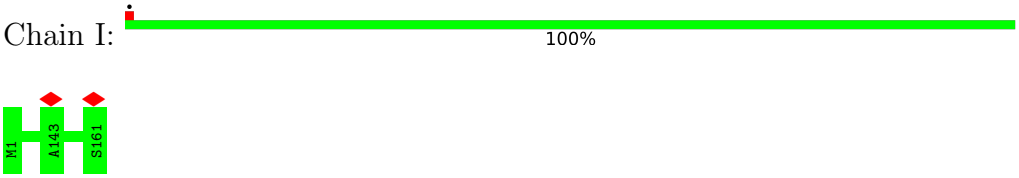
• Molecule 5: Allophycocyanin beta chain

Chain G:



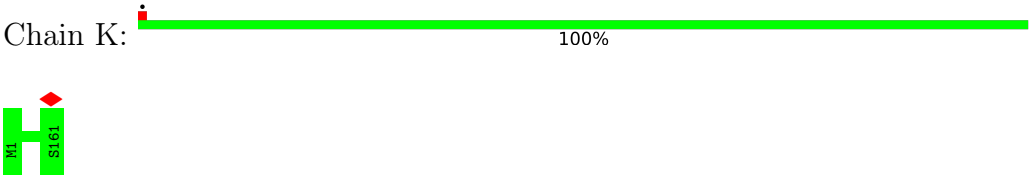
• Molecule 5: Allophycocyanin beta chain

Chain I:



• Molecule 5: Allophycocyanin beta chain

Chain K:



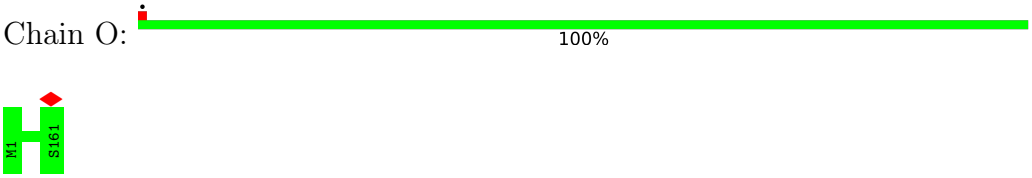
• Molecule 5: Allophycocyanin beta chain

Chain M:

There are no outlier residues recorded for this chain.

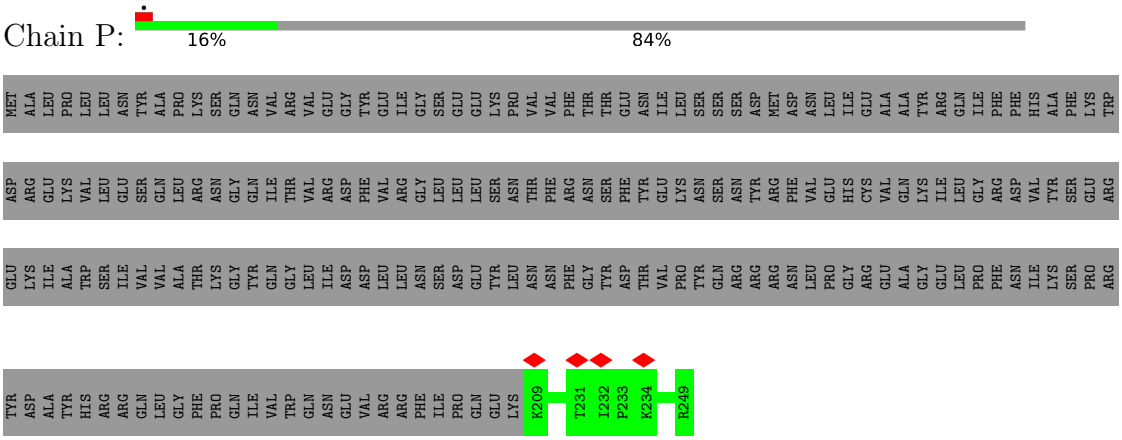
• Molecule 5: Allophycocyanin beta chain

Chain O:



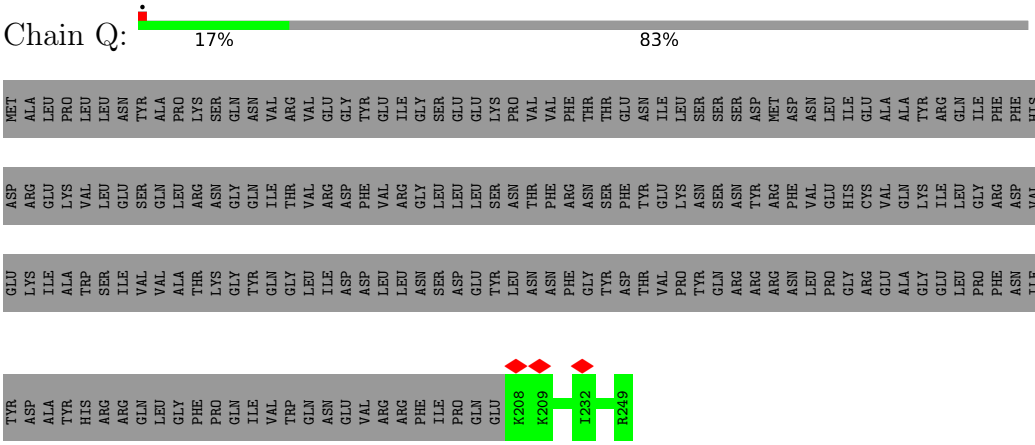
• Molecule 6: Phycobilisome rod-core linker polypeptide CpcG

Chain P:



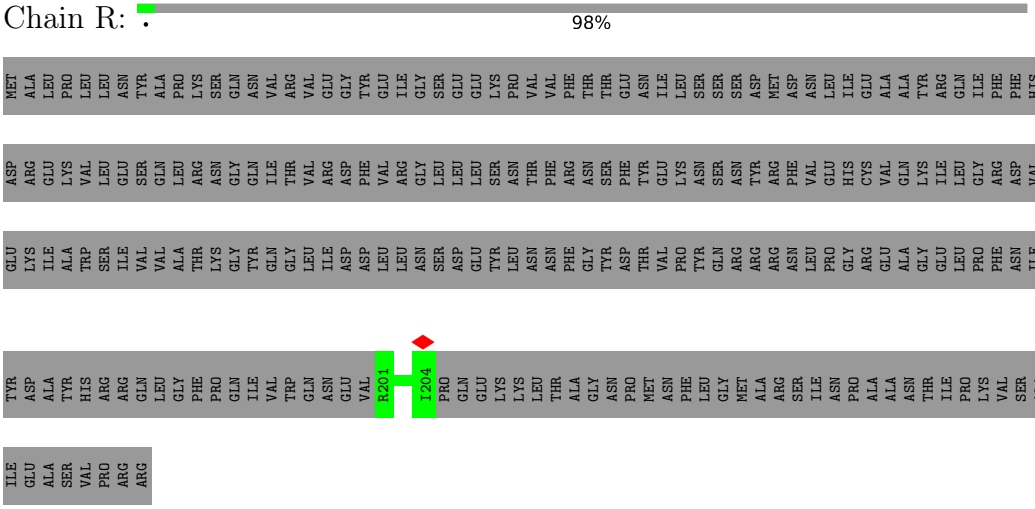
• Molecule 6: Phycobilisome rod-core linker polypeptide CpcG

Chain Q:



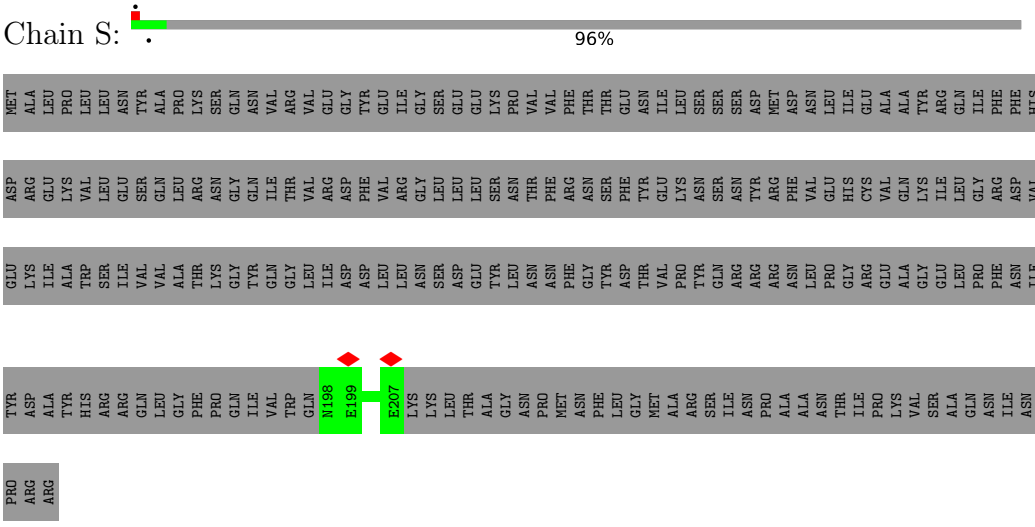
• Molecule 6: Phycobilisome rod-core linker polypeptide CpcG

Chain R:



• Molecule 6: Phycobilisome rod-core linker polypeptide CpcG

Chain S:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	153576	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	3.216	Depositor
Minimum map value	-1.526	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.083	Depositor
Recommended contour level	0.53	Depositor
Map size (Å)	372.224, 372.224, 372.224	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.727, 0.727, 0.727	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CYC, MEN, 45D

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.29	0/1727	0.51	0/2335
2	B	0.27	0/2327	0.47	0/3164
2	b	0.28	0/1047	0.49	0/1421
3	C	0.31	0/555	0.57	0/743
4	D	0.29	0/1225	0.52	0/1652
4	F	0.28	0/1225	0.51	0/1652
4	H	0.28	0/1225	0.50	0/1652
4	J	0.29	0/1225	0.51	0/1652
4	L	0.29	0/1225	0.51	0/1652
4	N	0.29	0/1225	0.51	0/1652
5	E	0.31	0/1211	0.48	0/1636
5	G	0.31	0/1211	0.48	0/1636
5	I	0.31	0/1211	0.48	0/1636
5	K	0.30	0/1211	0.49	0/1636
5	M	0.30	0/1211	0.48	0/1636
5	O	0.30	0/1211	0.48	0/1636
6	P	0.28	0/309	0.51	0/417
6	Q	0.27	0/318	0.53	0/428
6	R	0.28	0/41	0.80	0/52
6	S	0.30	0/91	0.62	0/121
All	All	0.29	0/21031	0.50	0/28409

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	208/896 (23%)	202 (97%)	6 (3%)	0	100	100
2	B	292/317 (92%)	282 (97%)	10 (3%)	0	100	100
2	b	128/317 (40%)	120 (94%)	8 (6%)	0	100	100
3	C	65/67 (97%)	65 (100%)	0	0	100	100
4	D	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
4	F	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
4	H	158/161 (98%)	158 (100%)	0	0	100	100
4	J	158/161 (98%)	158 (100%)	0	0	100	100
4	L	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
4	N	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
5	E	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
5	G	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
5	I	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
5	K	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
5	M	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
5	O	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
6	P	39/249 (16%)	39 (100%)	0	0	100	100
6	Q	40/249 (16%)	40 (100%)	0	0	100	100
6	R	2/249 (1%)	2 (100%)	0	0	100	100
6	S	8/249 (3%)	8 (100%)	0	0	100	100
All	All	2678/4525 (59%)	2631 (98%)	47 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	184/753 (24%)	183 (100%)	1 (0%)	88	92
2	B	239/257 (93%)	239 (100%)	0	100	100
2	b	112/257 (44%)	112 (100%)	0	100	100
3	C	58/58 (100%)	58 (100%)	0	100	100
4	D	128/129 (99%)	128 (100%)	0	100	100
4	F	128/129 (99%)	128 (100%)	0	100	100
4	H	128/129 (99%)	128 (100%)	0	100	100
4	J	128/129 (99%)	128 (100%)	0	100	100
4	L	128/129 (99%)	128 (100%)	0	100	100
4	N	128/129 (99%)	128 (100%)	0	100	100
5	E	124/124 (100%)	124 (100%)	0	100	100
5	G	124/124 (100%)	124 (100%)	0	100	100
5	I	124/124 (100%)	124 (100%)	0	100	100
5	K	124/124 (100%)	124 (100%)	0	100	100
5	M	124/124 (100%)	124 (100%)	0	100	100
5	O	124/124 (100%)	124 (100%)	0	100	100
6	P	33/221 (15%)	33 (100%)	0	100	100
6	Q	34/221 (15%)	34 (100%)	0	100	100
6	R	4/221 (2%)	4 (100%)	0	100	100
6	S	10/221 (4%)	10 (100%)	0	100	100
All	All	2186/3727 (59%)	2185 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	749	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	314	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	MEN	O	71	5	7,8,9	0.16	0	6,9,11	0.32	0
5	MEN	G	71	5	7,8,9	0.22	0	6,9,11	0.34	0
5	MEN	K	71	5	7,8,9	0.16	0	6,9,11	0.51	0
5	MEN	M	71	5	7,8,9	0.18	0	6,9,11	0.55	0
5	MEN	I	71	5	7,8,9	0.15	0	6,9,11	0.32	0
5	MEN	E	71	5	7,8,9	0.16	0	6,9,11	0.31	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MEN	O	71	5	-	2/7/8/10	-
5	MEN	G	71	5	-	2/7/8/10	-
5	MEN	K	71	5	-	2/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MEN	M	71	5	-	3/7/8/10	-
5	MEN	I	71	5	-	2/7/8/10	-
5	MEN	E	71	5	-	1/7/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	71	MEN	O-C-CA-CB
5	G	71	MEN	CA-CB-CG-OD1
5	I	71	MEN	CA-CB-CG-OD1
5	K	71	MEN	CA-CB-CG-ND2
5	K	71	MEN	CA-CB-CG-OD1
5	I	71	MEN	CA-CB-CG-ND2
5	G	71	MEN	CA-CB-CG-ND2
5	O	71	MEN	CA-CB-CG-ND2
5	O	71	MEN	CA-CB-CG-OD1
5	M	71	MEN	CA-CB-CG-OD1
5	E	71	MEN	CA-CB-CG-OD1
5	M	71	MEN	CA-CB-CG-ND2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	CYC	G	200	5	42,46,46	0.69	1 (2%)	50,67,67	0.63	2 (4%)
8	CYC	F	200	4	42,46,46	0.56	1 (2%)	50,67,67	0.85	3 (6%)
8	CYC	H	200	4	42,46,46	0.60	1 (2%)	50,67,67	0.79	3 (6%)
8	CYC	J	200	4	42,46,46	0.56	1 (2%)	50,67,67	0.89	2 (4%)
8	CYC	N	200	4	42,46,46	0.62	1 (2%)	50,67,67	0.91	3 (6%)
8	CYC	M	200	5	42,46,46	0.70	1 (2%)	50,67,67	0.80	3 (6%)
8	CYC	L	200	4	42,46,46	0.55	1 (2%)	50,67,67	0.99	3 (6%)
8	CYC	E	200	5	42,46,46	0.68	1 (2%)	50,67,67	0.63	2 (4%)
7	45D	B	400	-	43,43,43	0.98	1 (2%)	54,60,60	1.50	13 (24%)
8	CYC	O	200	5	42,46,46	0.55	1 (2%)	50,67,67	0.90	3 (6%)
8	CYC	I	200	5	42,46,46	0.66	1 (2%)	50,67,67	1.00	2 (4%)
8	CYC	D	200	4	42,46,46	0.51	1 (2%)	50,67,67	0.81	2 (4%)
8	CYC	K	200	5	42,46,46	0.58	1 (2%)	50,67,67	0.58	2 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	CYC	G	200	5	-	5/25/74/74	0/4/4/4
8	CYC	F	200	4	-	7/25/74/74	0/4/4/4
8	CYC	H	200	4	-	6/25/74/74	0/4/4/4
8	CYC	J	200	4	-	9/25/74/74	0/4/4/4
8	CYC	N	200	4	-	8/25/74/74	0/4/4/4
8	CYC	M	200	5	-	3/25/74/74	0/4/4/4
8	CYC	L	200	4	-	7/25/74/74	0/4/4/4
8	CYC	E	200	5	-	8/25/74/74	0/4/4/4
7	45D	B	400	-	-	11/29/69/69	0/2/2/2
8	CYC	O	200	5	-	6/25/74/74	0/4/4/4
8	CYC	I	200	5	-	3/25/74/74	0/4/4/4
8	CYC	D	200	4	-	7/25/74/74	0/4/4/4
8	CYC	K	200	5	-	6/25/74/74	0/4/4/4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	200	CYC	CHA-C1A	4.03	1.38	1.35
8	M	200	CYC	CHA-C1A	3.93	1.38	1.35
8	E	200	CYC	CHA-C1A	3.86	1.38	1.35
7	B	400	45D	C34-C36	3.50	1.53	1.45
8	I	200	CYC	CHA-C1A	3.39	1.38	1.35
8	K	200	CYC	CHA-C1A	3.20	1.37	1.35
8	H	200	CYC	CHA-C1A	3.08	1.37	1.35
8	N	200	CYC	CHA-C1A	3.07	1.37	1.35
8	J	200	CYC	CHA-C1A	2.86	1.37	1.35
8	F	200	CYC	CHA-C1A	2.74	1.37	1.35
8	L	200	CYC	CHA-C1A	2.69	1.37	1.35
8	O	200	CYC	CHA-C1A	2.61	1.37	1.35
8	D	200	CYC	CHA-C1A	2.35	1.37	1.35

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	I	200	CYC	C1B-CHB-C4A	4.99	140.26	128.08
8	L	200	CYC	C1B-CHB-C4A	4.92	140.10	128.08
8	J	200	CYC	C1B-CHB-C4A	4.47	139.01	128.08
8	N	200	CYC	C1B-CHB-C4A	4.46	138.98	128.08
8	O	200	CYC	C1B-CHB-C4A	4.14	138.19	128.08
8	F	200	CYC	C1B-CHB-C4A	4.05	137.98	128.08
8	D	200	CYC	C1B-CHB-C4A	3.84	137.47	128.08
8	H	200	CYC	C1B-CHB-C4A	3.54	136.72	128.08
8	M	200	CYC	C1B-CHB-C4A	3.10	135.65	128.08
7	B	400	45D	C05-C03-C07	3.00	115.10	110.48
8	L	200	CYC	CHA-C1A-NA	-2.86	124.85	128.83
8	G	200	CYC	CHA-C1A-NA	-2.85	124.87	128.83
8	O	200	CYC	CHA-C1A-NA	-2.78	124.96	128.83
7	B	400	45D	C39-C35-C33	2.78	122.45	118.08
8	M	200	CYC	CHA-C1A-NA	-2.73	125.04	128.83
8	I	200	CYC	CHA-C1A-NA	-2.72	125.05	128.83
7	B	400	45D	C21-C15-C07	-2.68	119.80	124.11
8	J	200	CYC	CHA-C1A-NA	-2.67	125.12	128.83
7	B	400	45D	C23-C19-C07	-2.66	119.74	127.20
8	H	200	CYC	CHA-C1A-NA	-2.58	125.24	128.83
7	B	400	45D	C40-C36-C34	2.53	122.07	118.08
7	B	400	45D	C20-C24-C26	-2.53	122.42	126.23
7	B	400	45D	C32-C30-C26	-2.52	123.72	127.31
8	E	200	CYC	CHA-C1A-NA	-2.49	125.37	128.83
7	B	400	45D	C22-C16-C08	-2.45	120.17	124.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	K	200	CYC	CHA-C1A-NA	-2.45	125.43	128.83
8	D	200	CYC	CHA-C1A-NA	-2.38	125.52	128.83
7	B	400	45D	C39-C35-C37	-2.36	119.62	122.92
8	F	200	CYC	CHA-C1A-NA	-2.34	125.58	128.83
8	M	200	CYC	C2C-C3C-C4C	2.33	104.82	101.34
7	B	400	45D	C06-C04-C08	2.30	114.02	110.48
7	B	400	45D	C22-C16-C18	2.28	118.86	115.48
8	N	200	CYC	CHA-C1A-NA	-2.25	125.70	128.83
8	N	200	CYC	C2C-C3C-C4C	2.22	104.66	101.34
8	L	200	CYC	C2C-C3C-C4C	2.20	104.63	101.34
8	O	200	CYC	C2C-C3C-C4C	2.19	104.61	101.34
8	E	200	CYC	C2C-C3C-C4C	2.15	104.56	101.34
7	B	400	45D	C41-C42-C38	-2.14	119.10	123.47
7	B	400	45D	C32-C34-C36	-2.13	120.44	126.42
8	K	200	CYC	C2C-C3C-C4C	2.09	104.48	101.34
8	F	200	CYC	C2C-C3C-C4C	2.09	104.47	101.34
8	G	200	CYC	C2C-C3C-C4C	2.09	104.47	101.34
8	H	200	CYC	C2C-C3C-C4C	2.07	104.43	101.34

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	400	45D	C03-C07-C19-C23
7	B	400	45D	C15-C07-C19-C23
7	B	400	45D	C16-C08-C20-C24
7	B	400	45D	C20-C24-C26-C28
7	B	400	45D	C20-C24-C26-C30
7	B	400	45D	C32-C34-C36-C38
7	B	400	45D	C32-C34-C36-C40
8	E	200	CYC	NA-C4A-CHB-C1B
8	E	200	CYC	C3A-C4A-CHB-C1B
8	E	200	CYC	ND-C1D-CHD-C4C
8	G	200	CYC	NA-C4A-CHB-C1B
8	G	200	CYC	C3A-C4A-CHB-C1B
8	G	200	CYC	ND-C1D-CHD-C4C
8	J	200	CYC	C4B-C3B-CAB-CBB
8	K	200	CYC	NA-C4A-CHB-C1B
8	K	200	CYC	C3A-C4A-CHB-C1B
8	K	200	CYC	ND-C1D-CHD-C4C
8	M	200	CYC	NA-C4A-CHB-C1B
8	M	200	CYC	C3A-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
8	N	200	CYC	C4B-C3B-CAB-CBB
8	O	200	CYC	ND-C1D-CHD-C4C
8	O	200	CYC	C2D-C1D-CHD-C4C
8	H	200	CYC	NA-C4A-CHB-C1B
7	B	400	45D	C19-C23-C25-C27
7	B	400	45D	C19-C23-C25-C29
8	N	200	CYC	C2B-C3B-CAB-CBB
8	D	200	CYC	NA-C4A-CHB-C1B
8	F	200	CYC	NA-C4A-CHB-C1B
8	I	200	CYC	NA-C4A-CHB-C1B
8	J	200	CYC	NA-C4A-CHB-C1B
8	L	200	CYC	NA-C4A-CHB-C1B
8	N	200	CYC	NA-C4A-CHB-C1B
8	O	200	CYC	NA-C4A-CHB-C1B
8	D	200	CYC	C3A-C4A-CHB-C1B
8	F	200	CYC	C3A-C4A-CHB-C1B
8	H	200	CYC	C3A-C4A-CHB-C1B
8	I	200	CYC	C3A-C4A-CHB-C1B
8	J	200	CYC	C3A-C4A-CHB-C1B
8	L	200	CYC	C3A-C4A-CHB-C1B
8	N	200	CYC	C3A-C4A-CHB-C1B
8	O	200	CYC	C3A-C4A-CHB-C1B
7	B	400	45D	C04-C08-C20-C24
8	J	200	CYC	C2B-C3B-CAB-CBB
8	L	200	CYC	C4B-C3B-CAB-CBB
8	J	200	CYC	C2A-CAA-CBA-CGA
8	E	200	CYC	C2B-C3B-CAB-CBB
7	B	400	45D	C26-C30-C32-C34
8	E	200	CYC	CAD-CBD-CGD-O1D
8	L	200	CYC	CAA-CBA-CGA-O2A
8	O	200	CYC	CAD-CBD-CGD-O1D
8	G	200	CYC	CAD-CBD-CGD-O1D
8	H	200	CYC	CAA-CBA-CGA-O1A
8	F	200	CYC	CAA-CBA-CGA-O1A
8	E	200	CYC	CAA-CBA-CGA-O2A
8	E	200	CYC	CAD-CBD-CGD-O2D
8	E	200	CYC	CAA-CBA-CGA-O1A
8	F	200	CYC	CAA-CBA-CGA-O2A
8	J	200	CYC	CAD-CBD-CGD-O1D
8	D	200	CYC	CAA-CBA-CGA-O1A
8	F	200	CYC	CAD-CBD-CGD-O1D
8	H	200	CYC	CAA-CBA-CGA-O2A

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Continued from previous page...

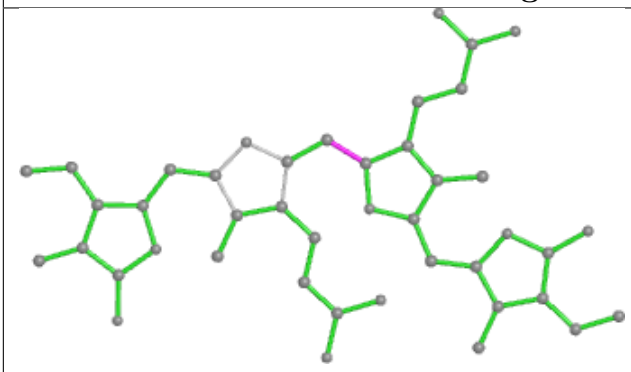
Mol	Chain	Res	Type	Atoms
8	J	200	CYC	CAD-CBD-CGD-O2D
8	L	200	CYC	CAA-CBA-CGA-O1A
8	G	200	CYC	CAD-CBD-CGD-O2D
8	K	200	CYC	C3A-C2A-CAA-CBA
8	D	200	CYC	CAA-CBA-CGA-O2A
8	F	200	CYC	C2A-CAA-CBA-CGA
8	O	200	CYC	CAD-CBD-CGD-O2D
8	K	200	CYC	C2B-C3B-CAB-CBB
8	J	200	CYC	CAA-CBA-CGA-O2A
8	D	200	CYC	CAD-CBD-CGD-O1D
8	J	200	CYC	CAA-CBA-CGA-O1A
8	L	200	CYC	CAD-CBD-CGD-O1D
8	L	200	CYC	CAD-CBD-CGD-O2D
8	F	200	CYC	CAD-CBD-CGD-O2D
8	H	200	CYC	CAD-CBD-CGD-O1D
8	N	200	CYC	CAA-CBA-CGA-O1A
8	N	200	CYC	CAA-CBA-CGA-O2A
8	N	200	CYC	CAD-CBD-CGD-O1D
8	H	200	CYC	CAD-CBD-CGD-O2D
8	D	200	CYC	C2A-CAA-CBA-CGA
8	D	200	CYC	CAD-CBD-CGD-O2D
8	N	200	CYC	CAD-CBD-CGD-O2D
8	I	200	CYC	CAD-CBD-CGD-O2D
8	M	200	CYC	CAA-CBA-CGA-O2A
8	K	200	CYC	CAA-CBA-CGA-O2A

There are no ring outliers.

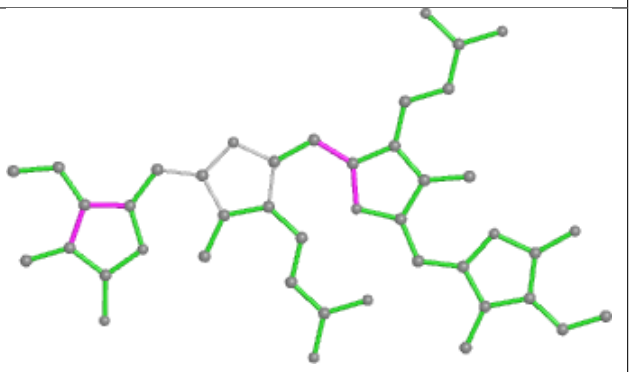
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

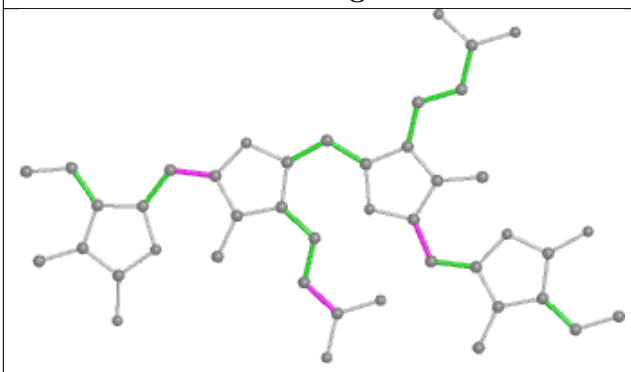
Ligand CYC G 200



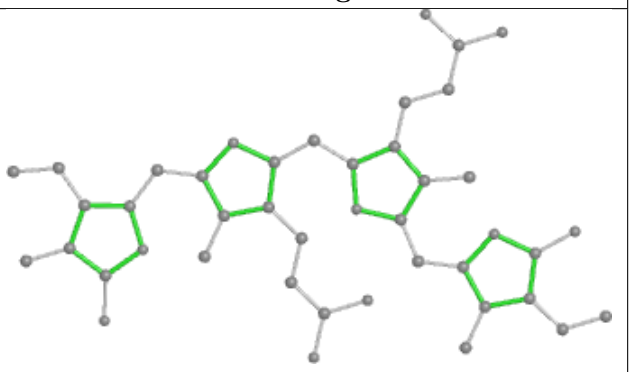
Bond lengths



Bond angles

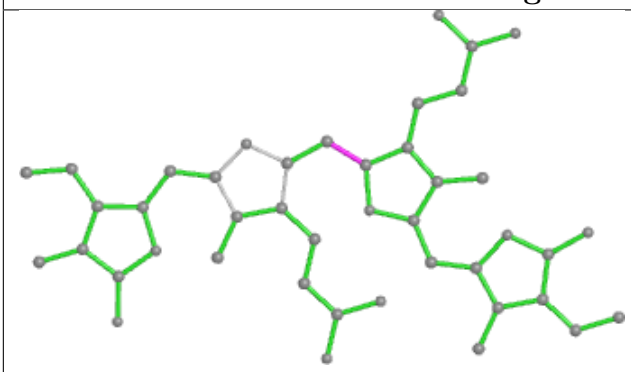


Torsions

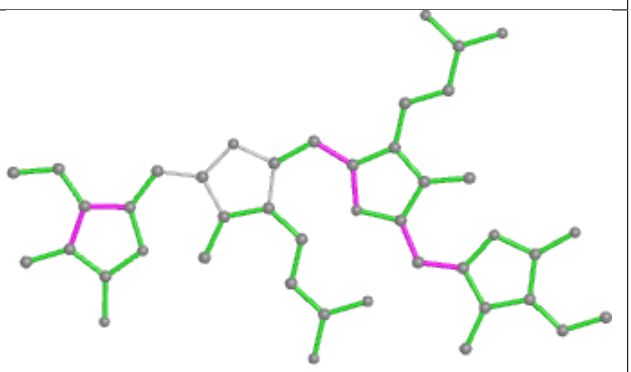


Rings

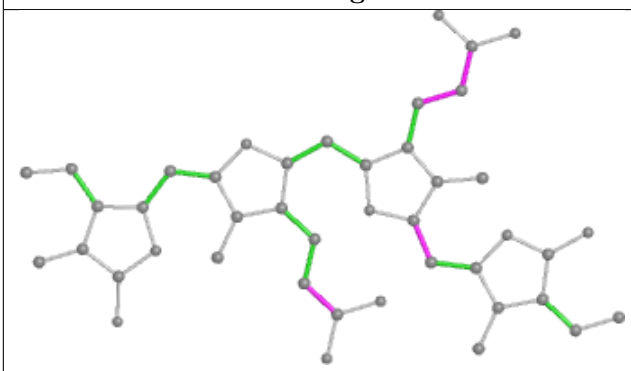
Ligand CYC F 200



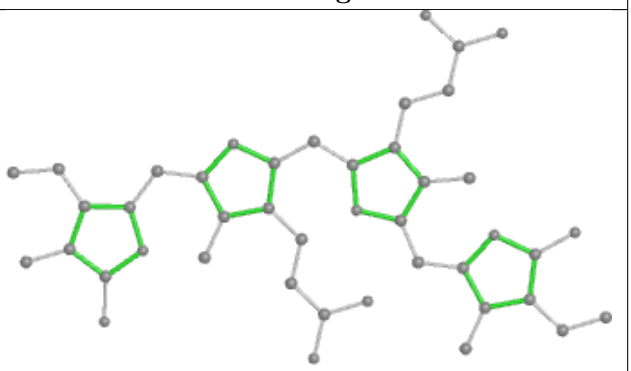
Bond lengths



Bond angles

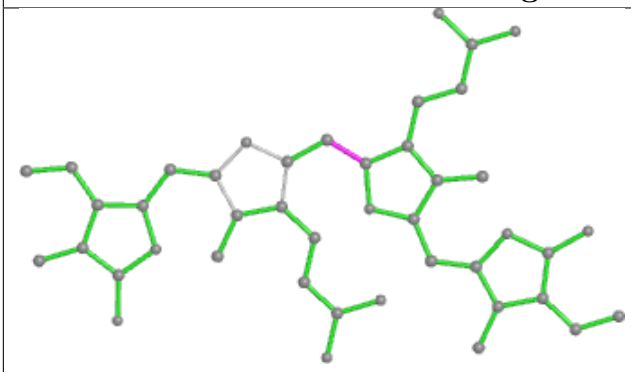


Torsions

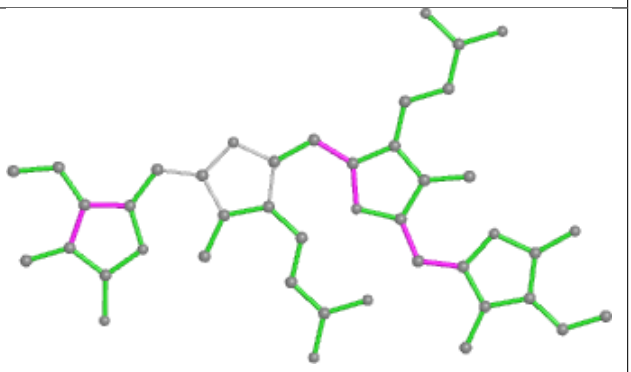


Rings

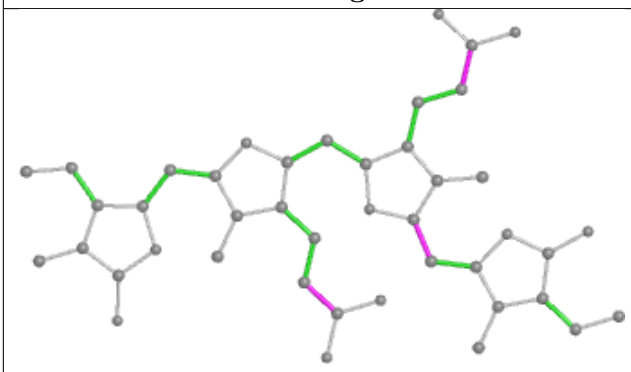
Ligand CYC H 200



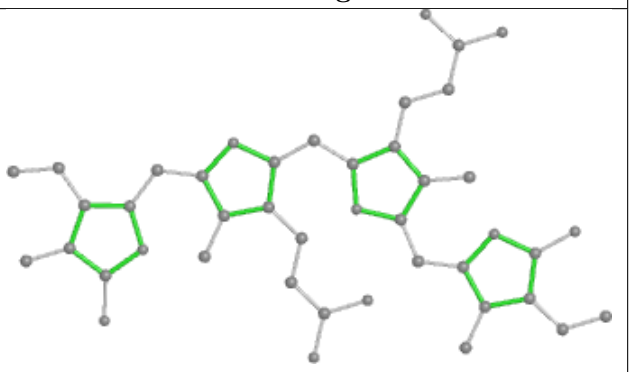
Bond lengths



Bond angles

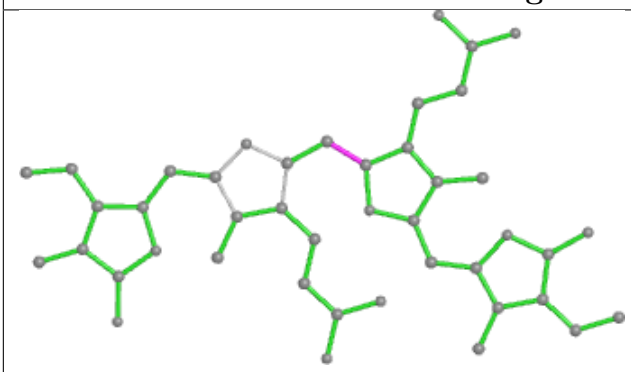


Torsions

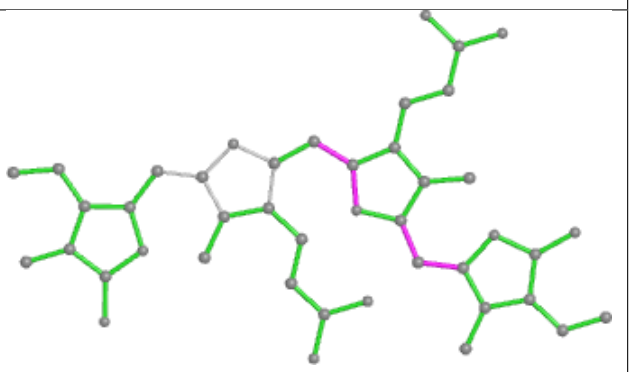


Rings

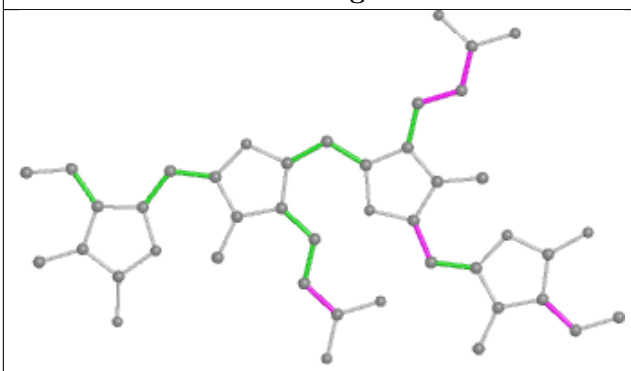
Ligand CYC J 200



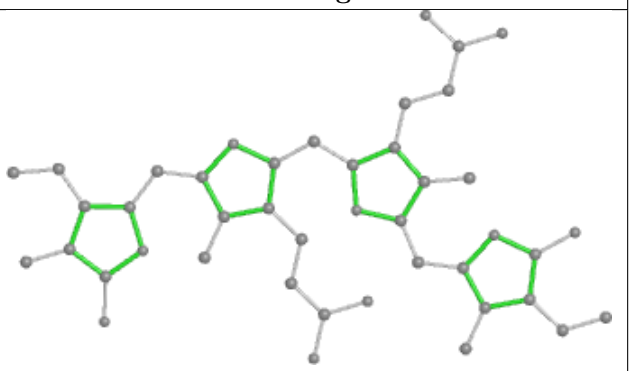
Bond lengths



Bond angles

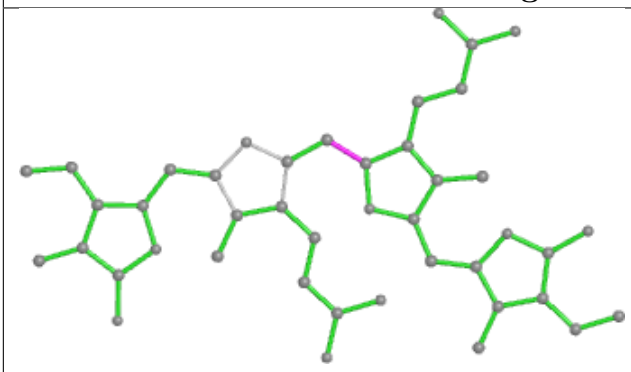


Torsions

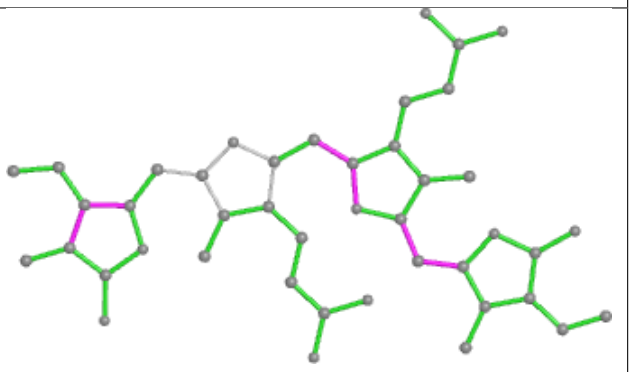


Rings

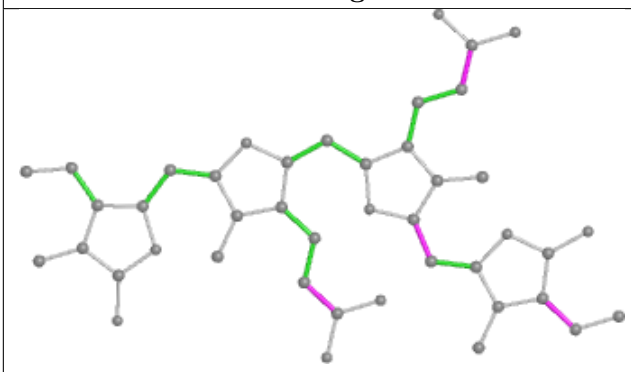
Ligand CYC N 200



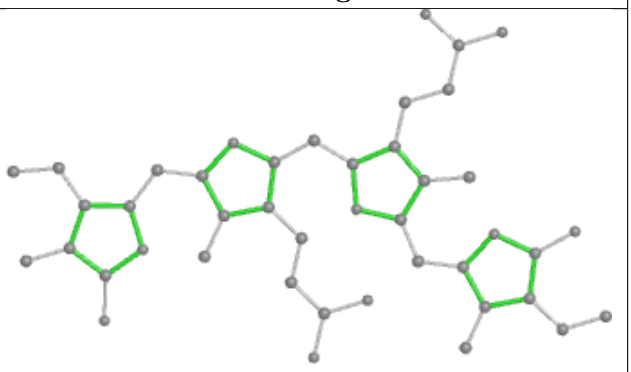
Bond lengths



Bond angles

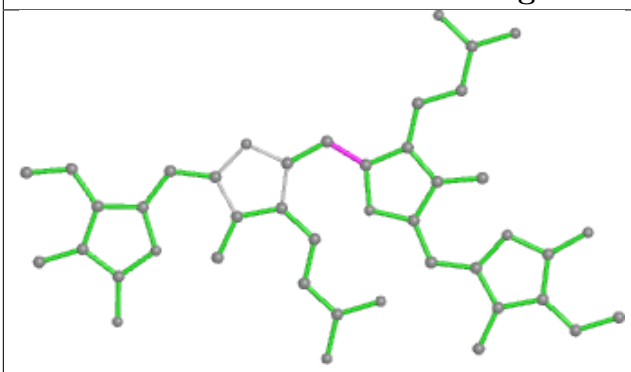


Torsions

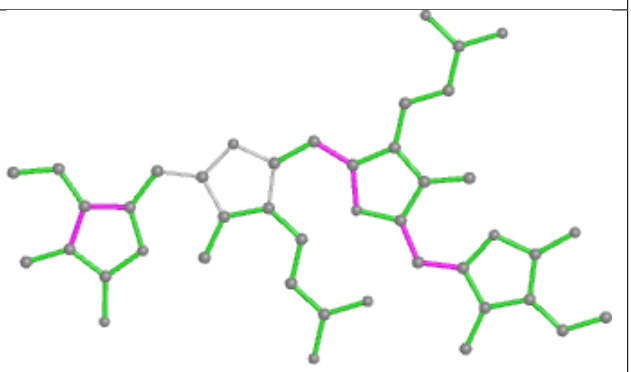


Rings

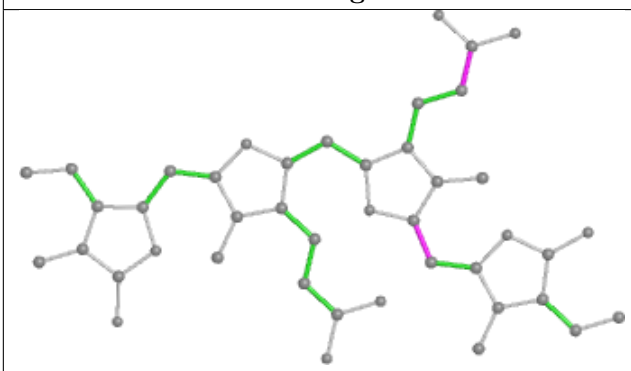
Ligand CYC M 200



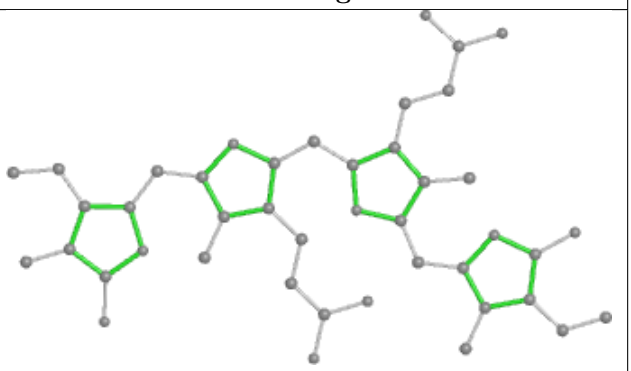
Bond lengths



Bond angles

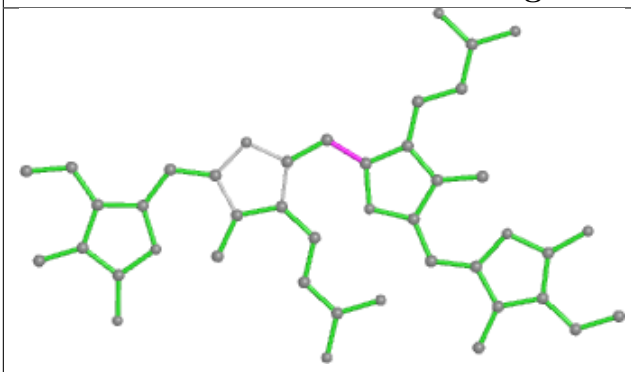


Torsions

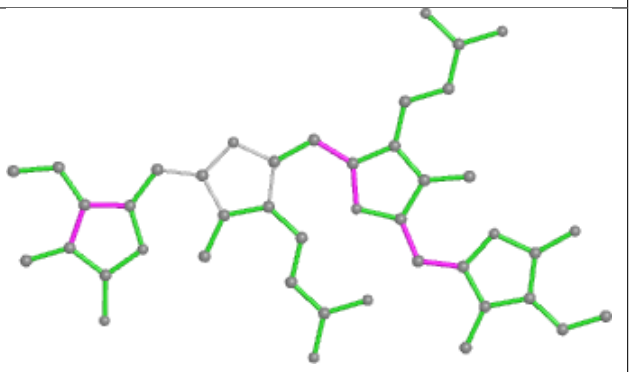


Rings

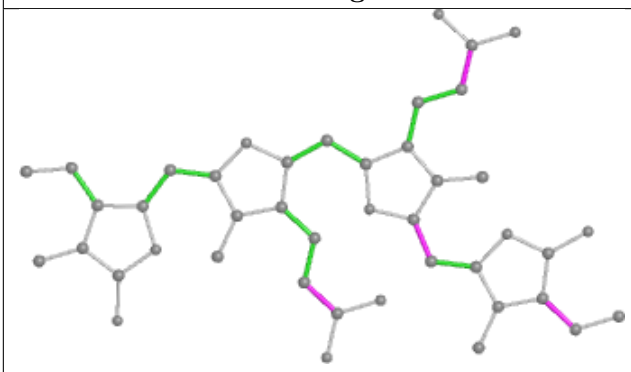
Ligand CYC L 200



Bond lengths



Bond angles



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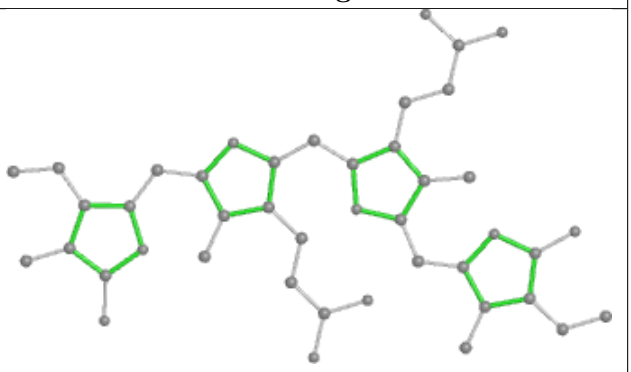
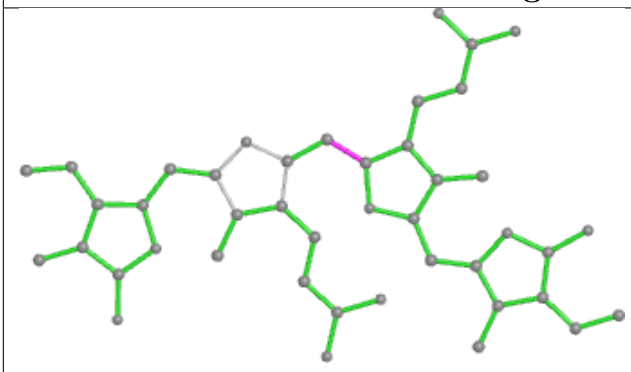
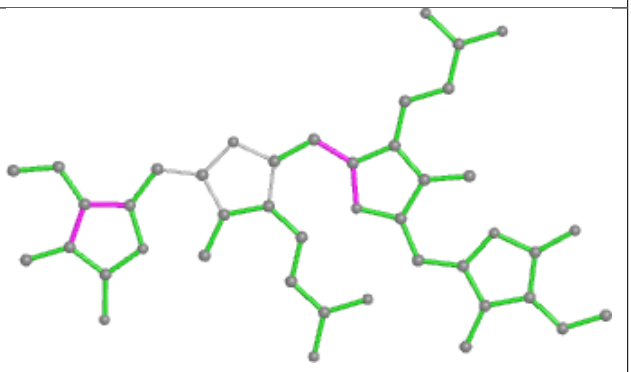


Rings

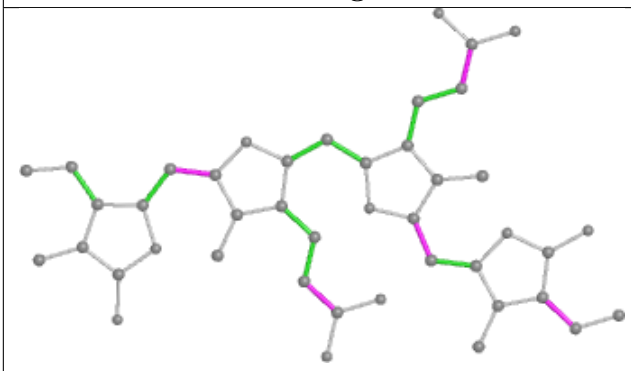
Ligand CYC E 200



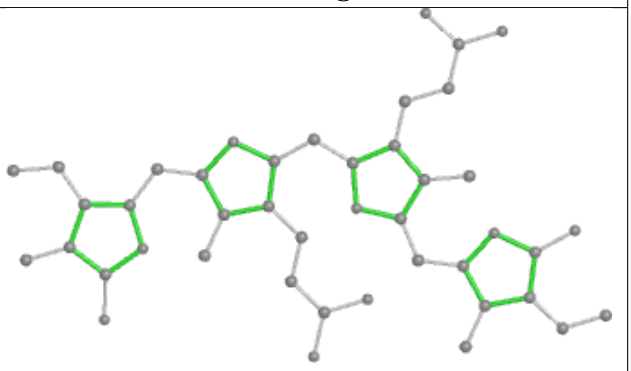
Bond lengths



Bond angles

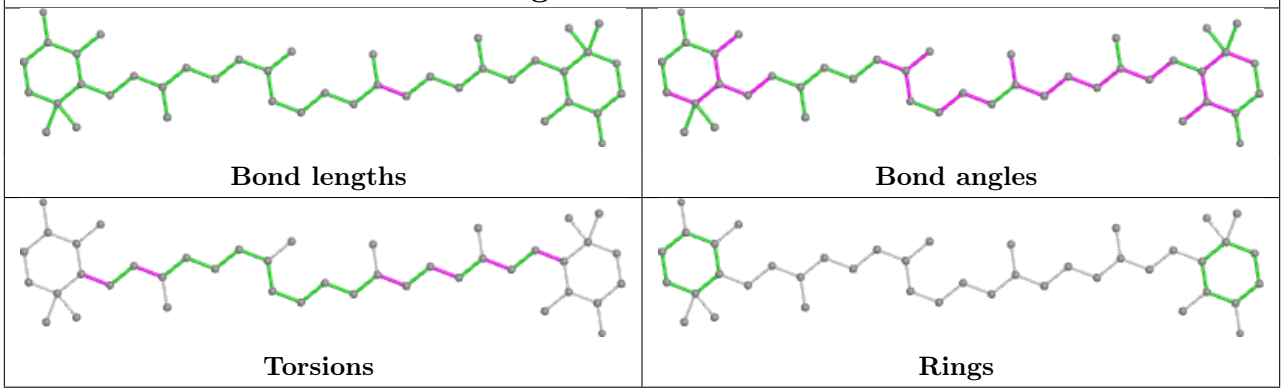


Torsions

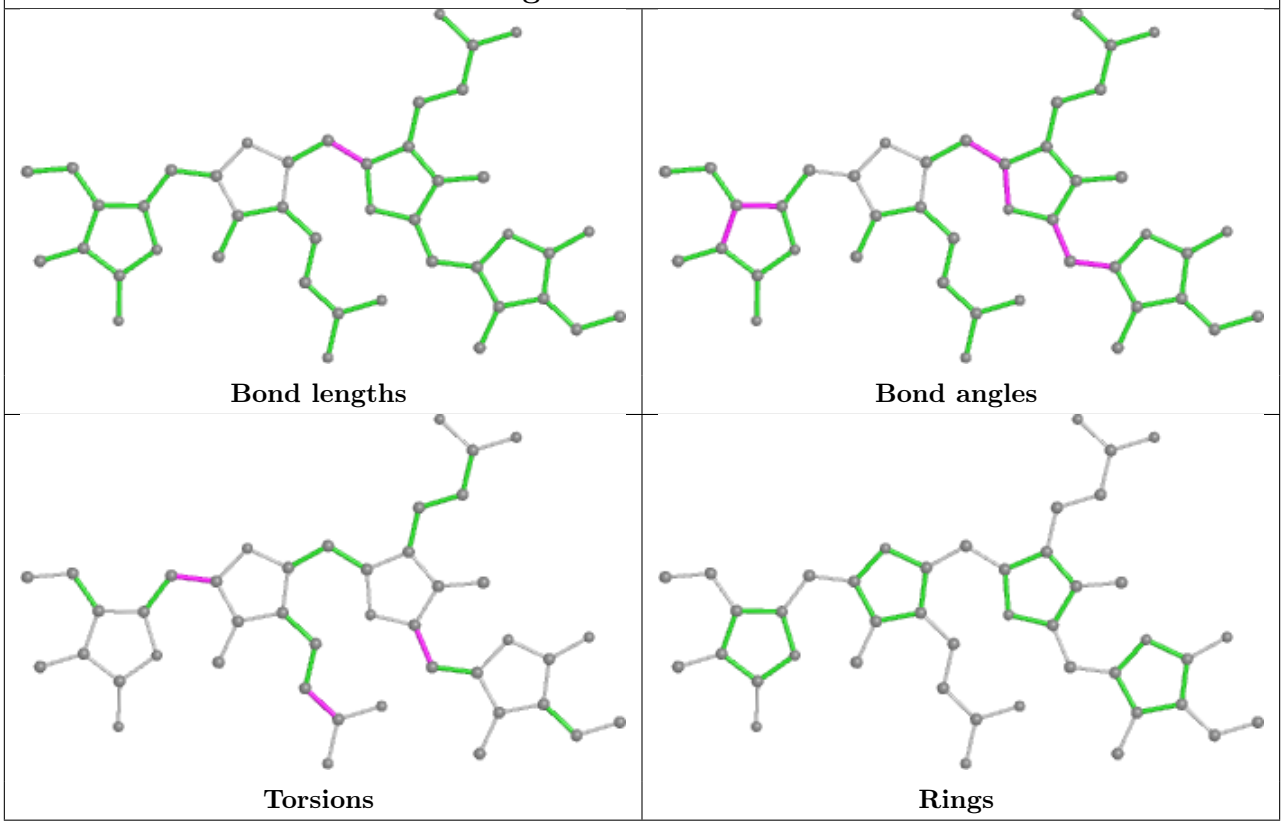


Rings

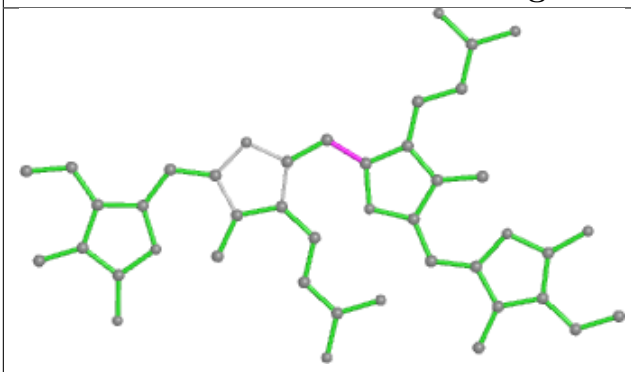
Ligand 45D B 400



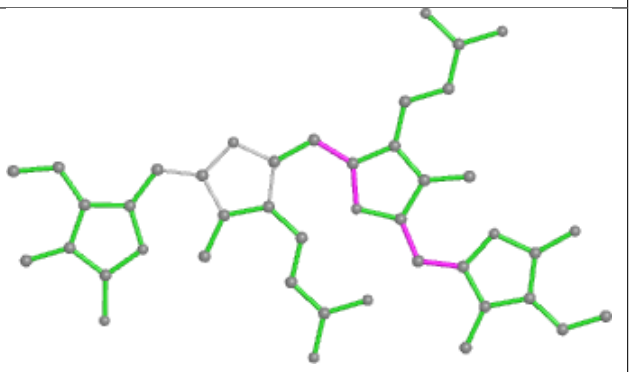
Ligand CYC O 200



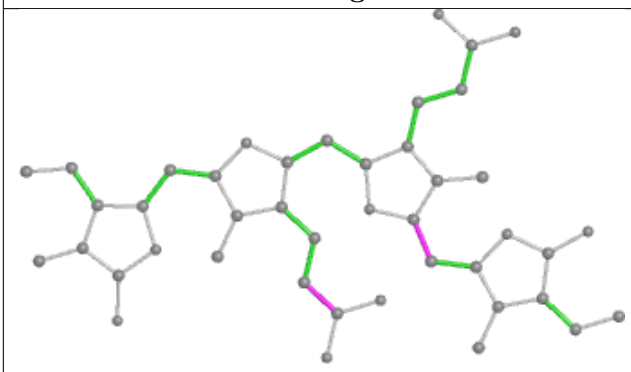
Ligand CYC I 200



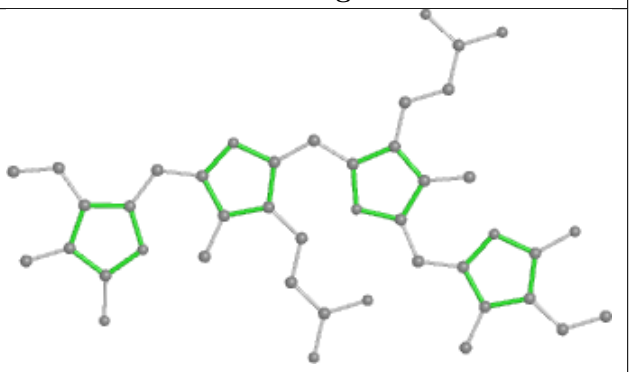
Bond lengths



Bond angles

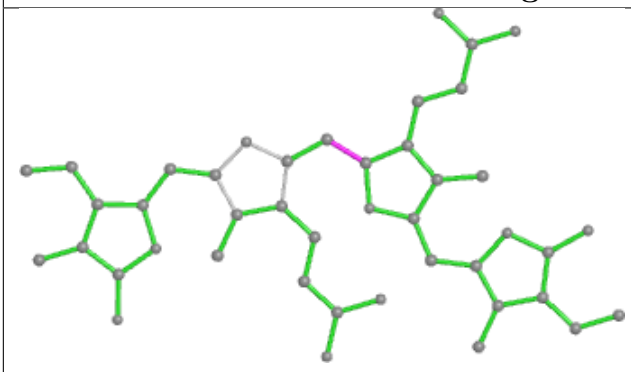


Torsions

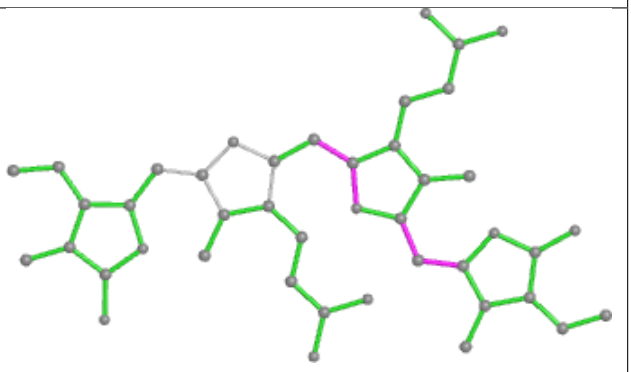


Rings

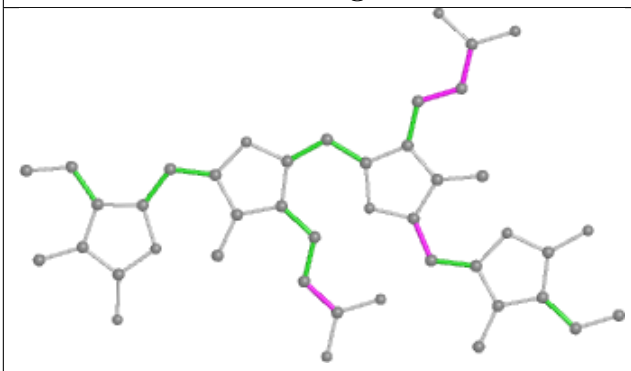
Ligand CYC D 200



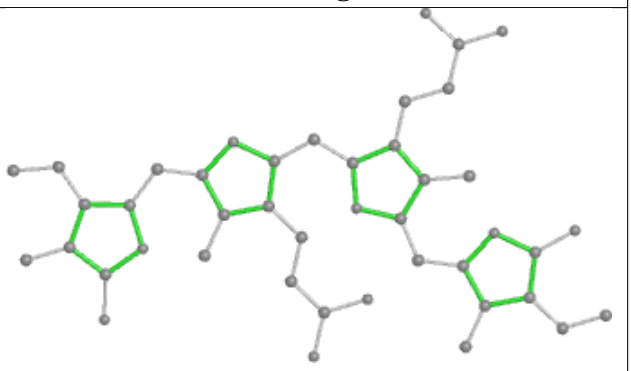
Bond lengths



Bond angles

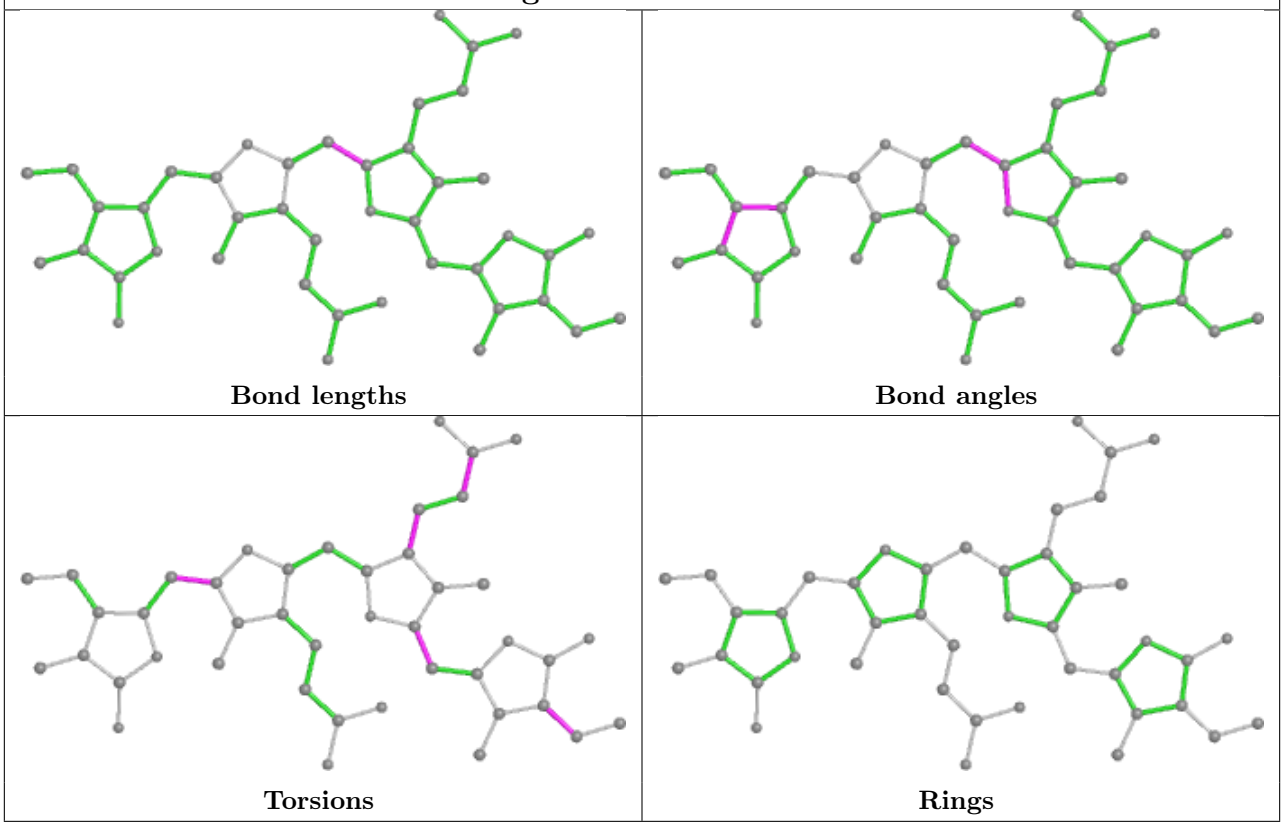


Torsions



Rings

Ligand CYC K 200



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

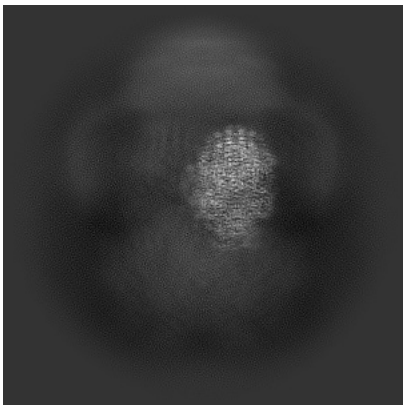
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41475. These allow visual inspection of the internal detail of the map and identification of artifacts.

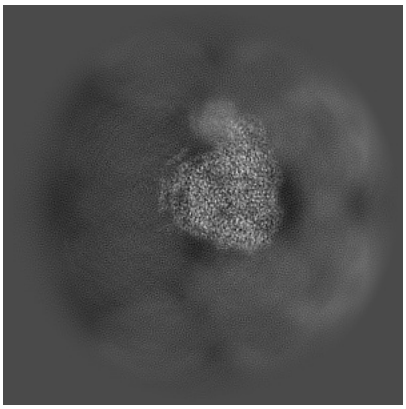
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

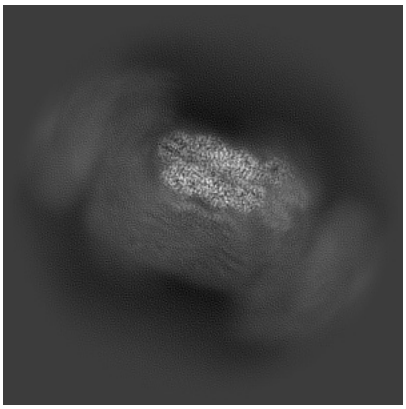
6.1.1 Primary map



X

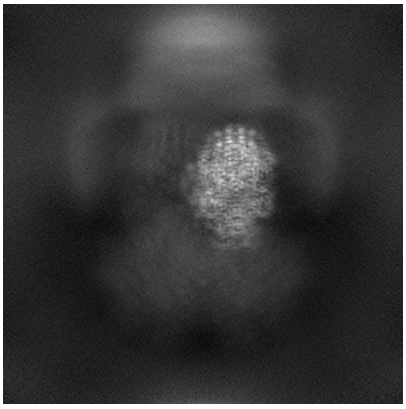


Y

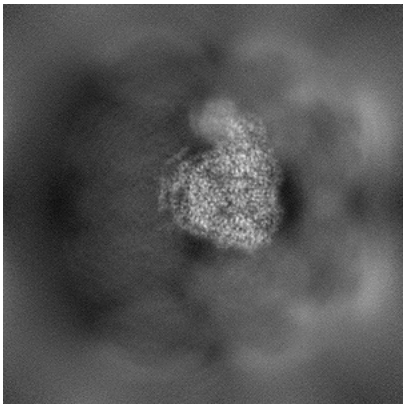


Z

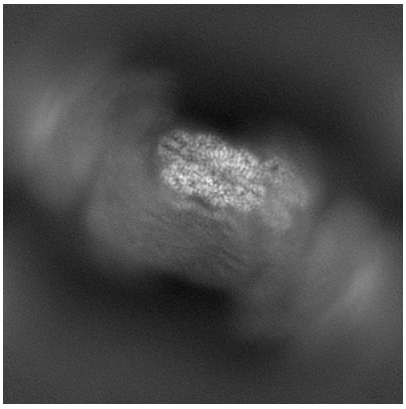
6.1.2 Raw map



X



Y

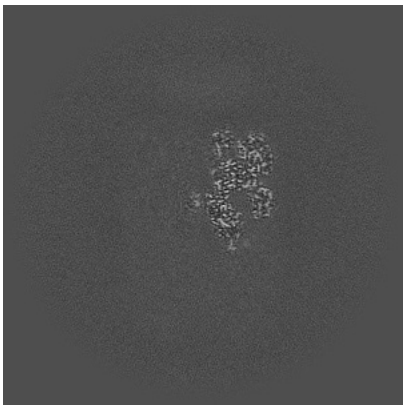


Z

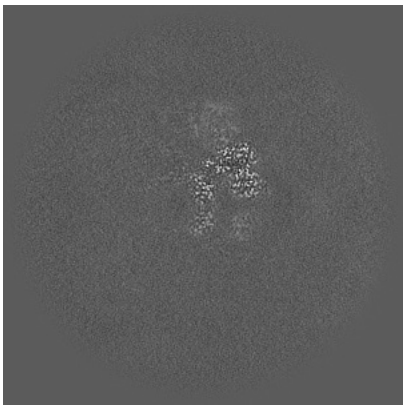
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

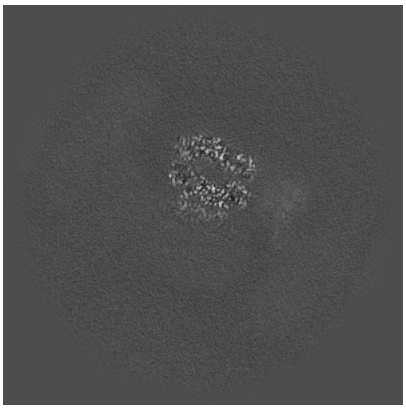
6.2.1 Primary map



X Index: 256

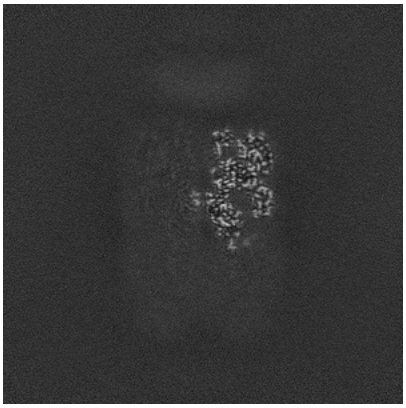


Y Index: 256

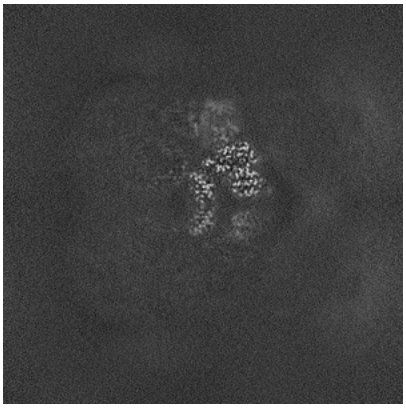


Z Index: 256

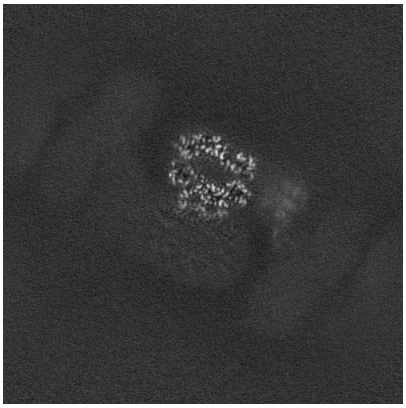
6.2.2 Raw map



X Index: 256



Y Index: 256

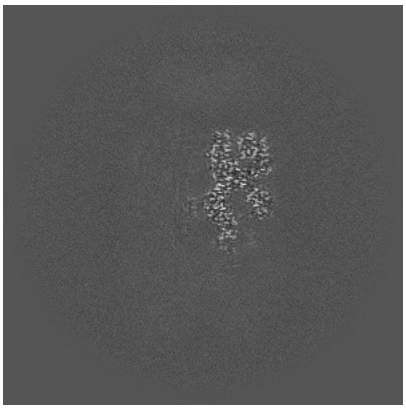


Z Index: 256

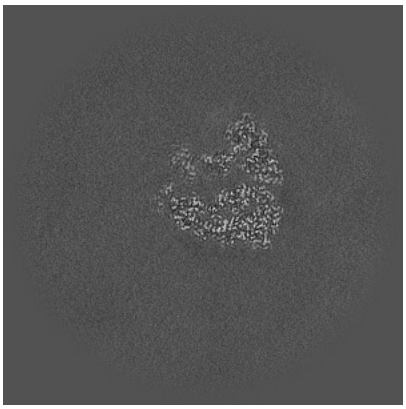
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

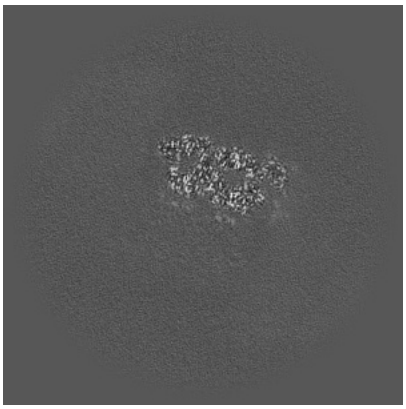
6.3.1 Primary map



X Index: 261

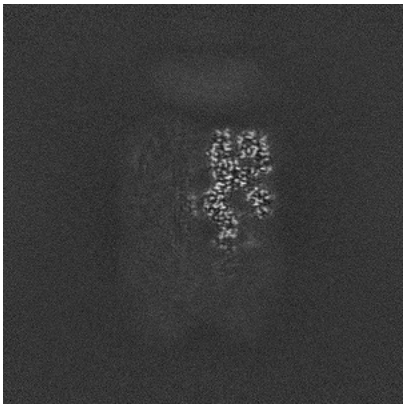


Y Index: 290

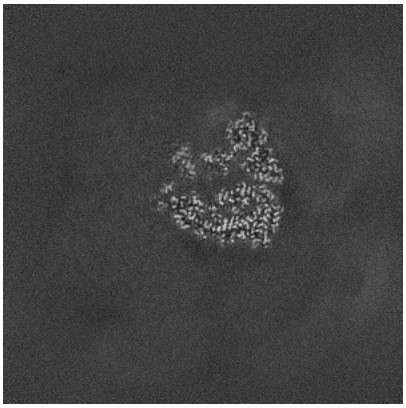


Z Index: 299

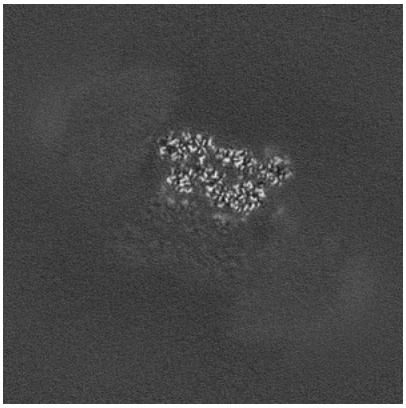
6.3.2 Raw map



X Index: 261



Y Index: 290

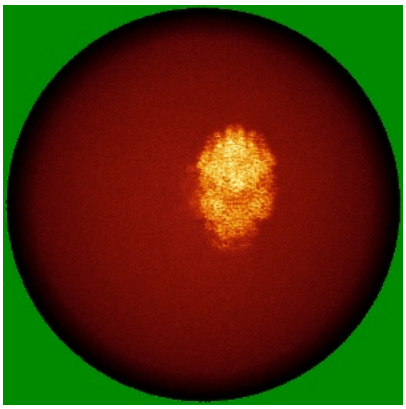


Z Index: 306

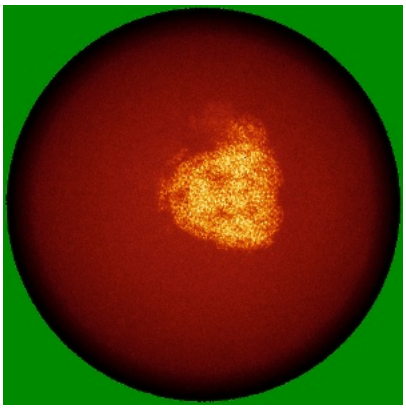
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

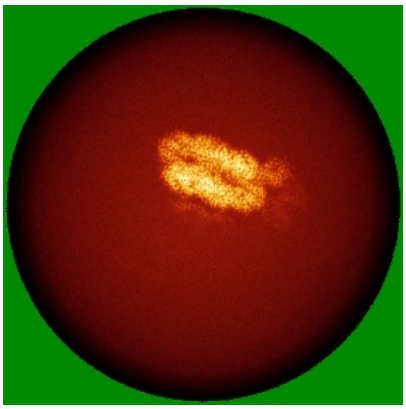
6.4.1 Primary map



X

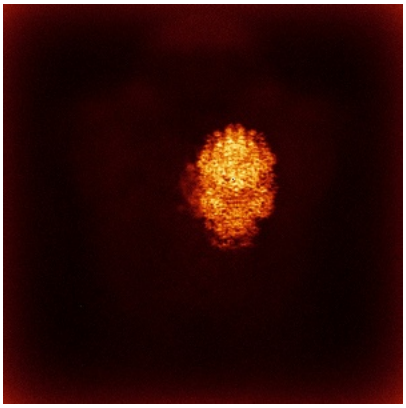


Y

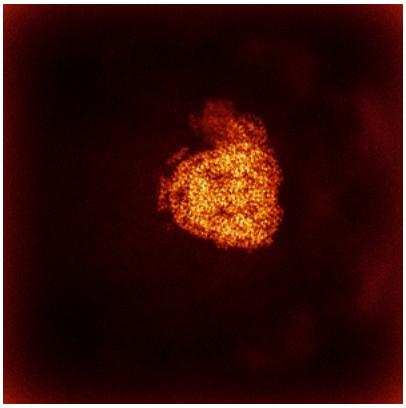


Z

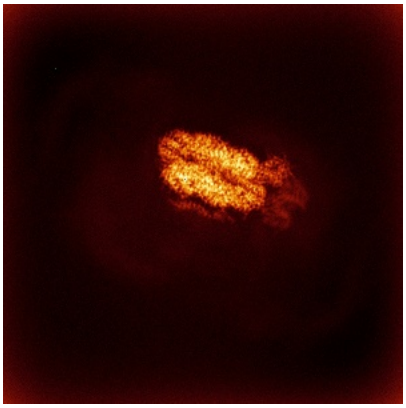
6.4.2 Raw map



X



Y

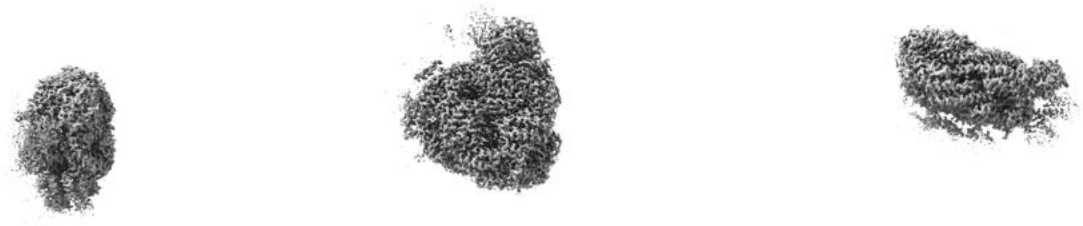


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

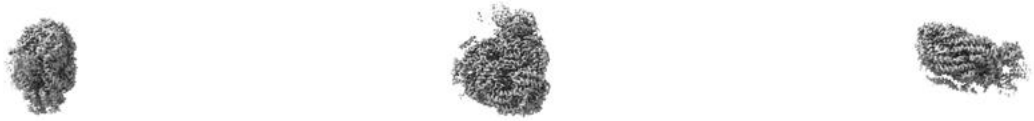
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.53. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

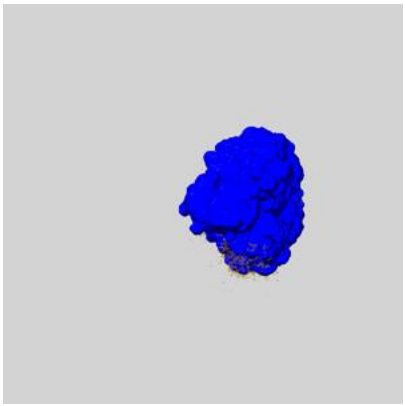
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

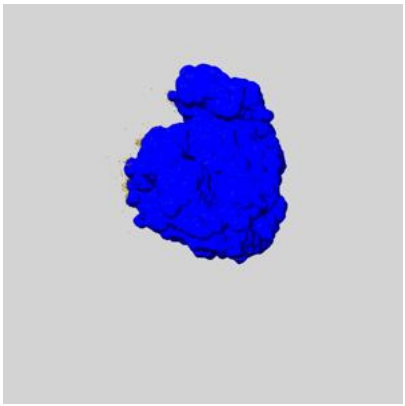
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

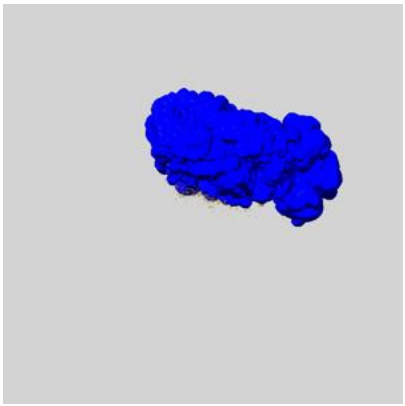
6.6.1 emd_41475_msk_1.map (i)



X



Y

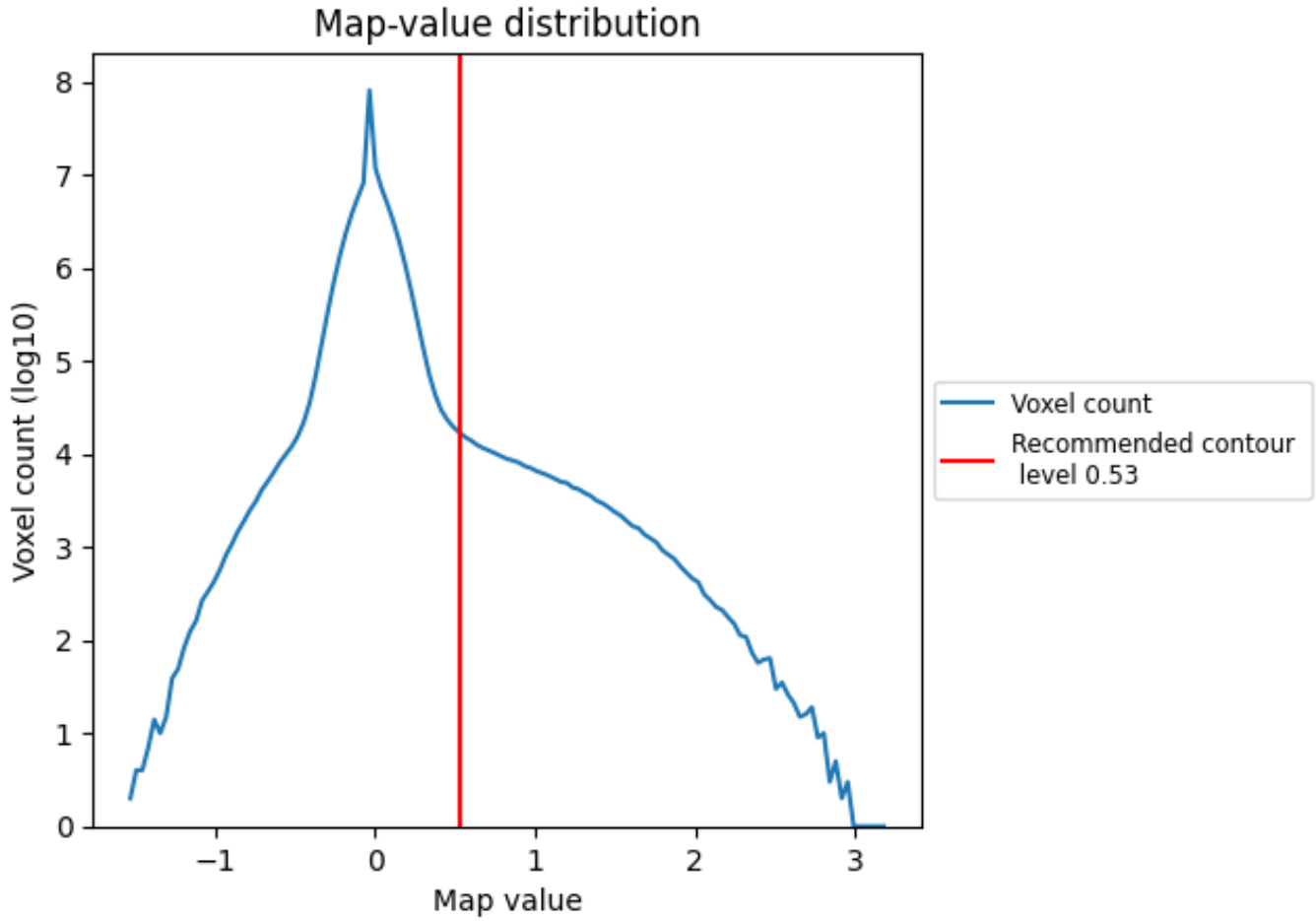


Z

7 Map analysis

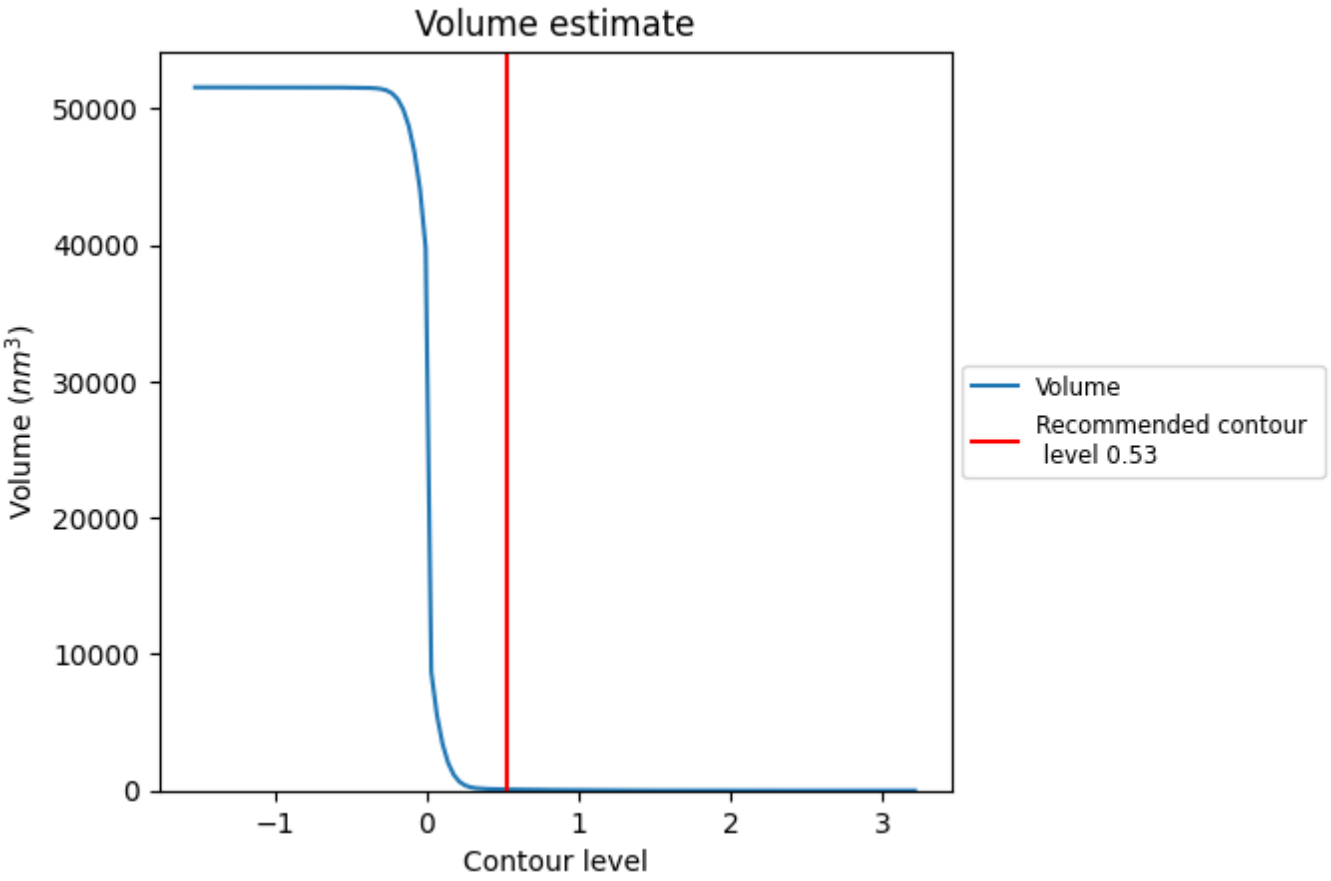
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

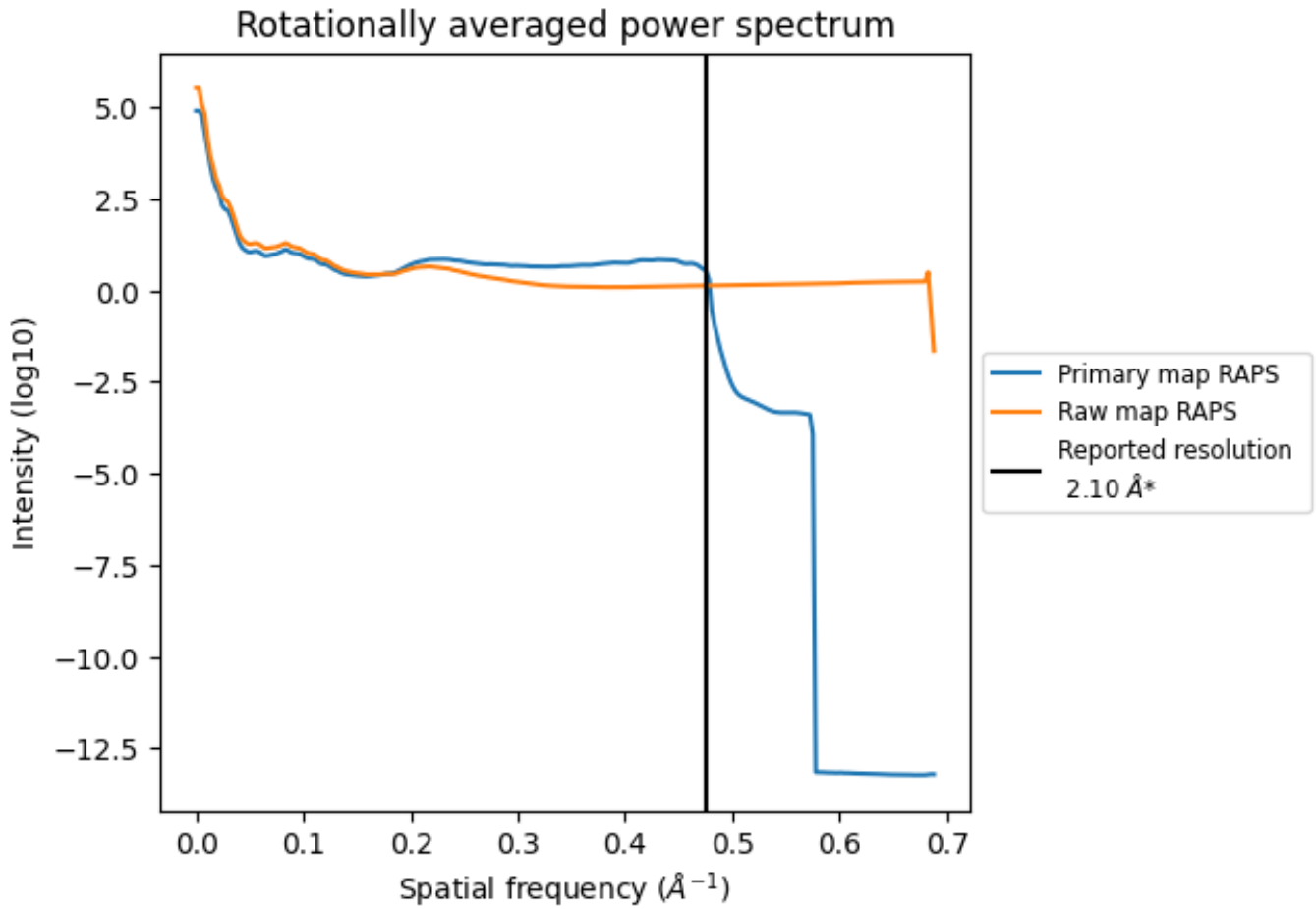
7.2 Volume estimate



The volume at the recommended contour level is 84 nm^3; this corresponds to an approximate mass of 76 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

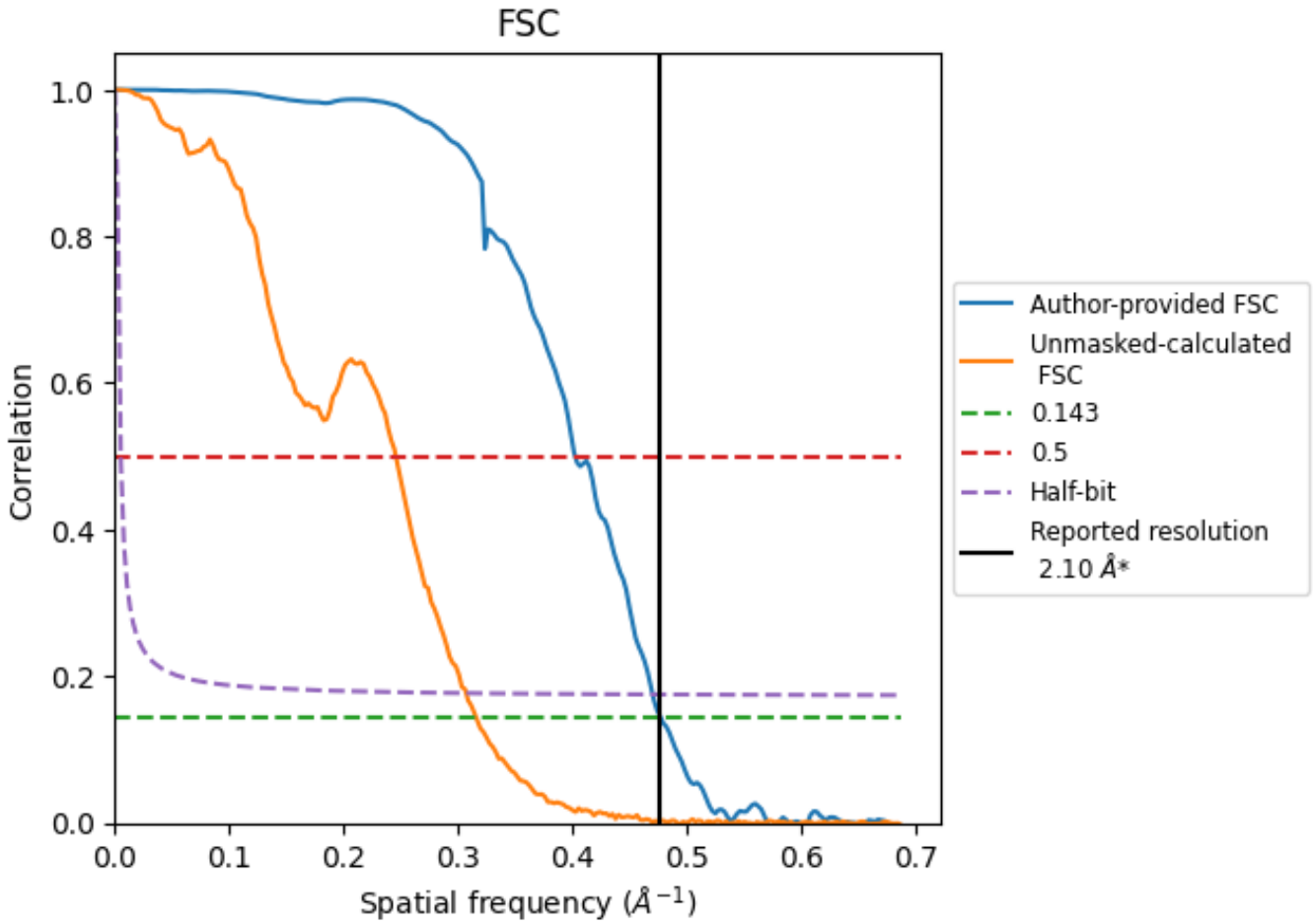


*Reported resolution corresponds to spatial frequency of 0.476 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.476 Å^{-1}

8.2 Resolution estimates (i)

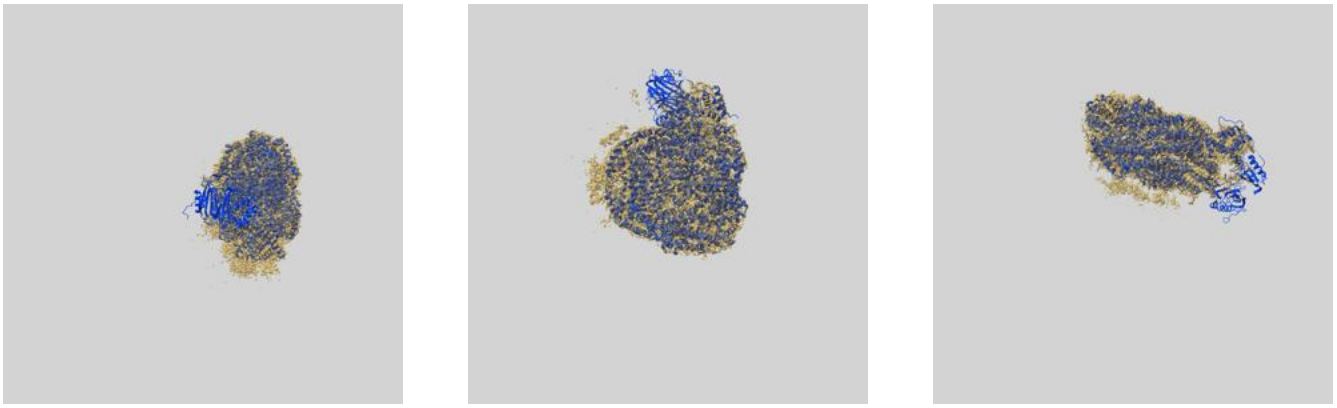
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.10	-	-
Author-provided FSC curve	2.09	2.48	2.13
Unmasked-calculated*	3.16	4.07	3.26

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.16 differs from the reported value 2.1 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41475 and PDB model 8TPJ. Per-residue inclusion information can be found in section 3 on page 9.

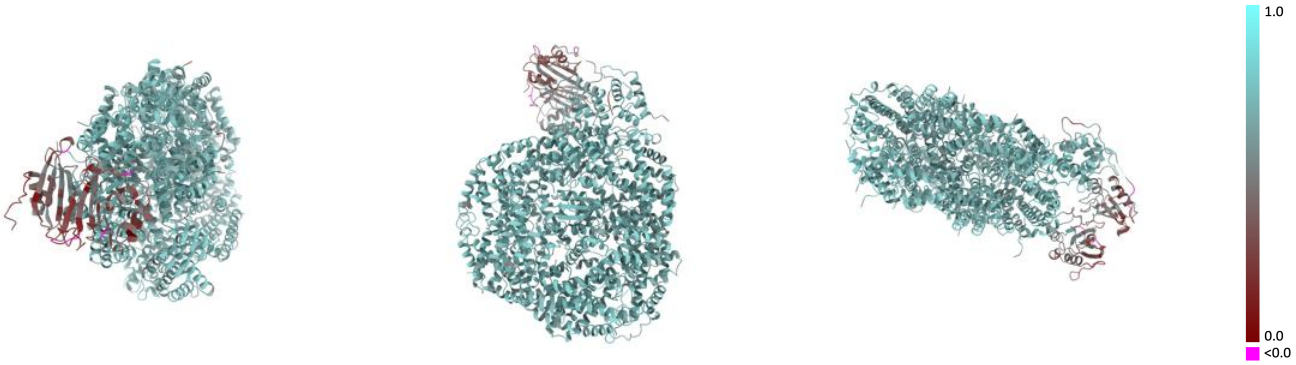
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.53 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

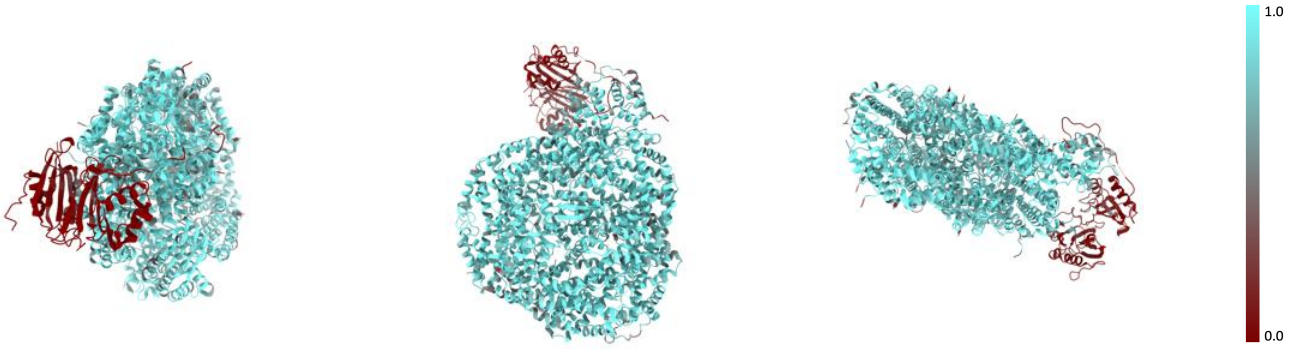
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

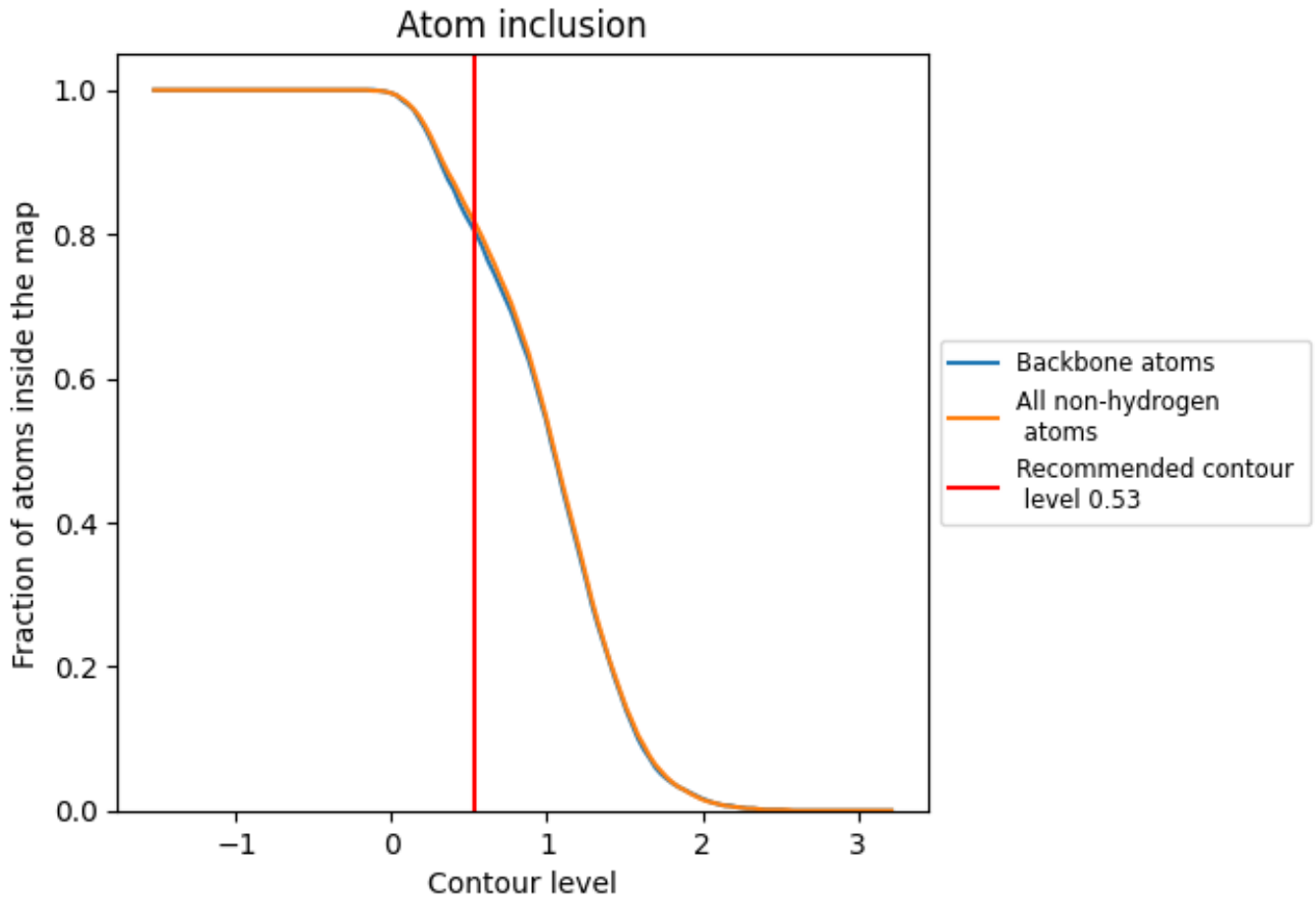
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.53).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.53) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8180	0.6750
A	0.9340	0.7270
B	0.4480	0.5250
C	0.9220	0.7110
D	0.9130	0.7000
E	0.9170	0.7020
F	0.8920	0.6970
G	0.9110	0.7050
H	0.8950	0.7020
I	0.9340	0.7170
J	0.9150	0.7030
K	0.9320	0.7250
L	0.9110	0.7210
M	0.9440	0.7310
N	0.9230	0.7170
O	0.9290	0.7120
P	0.7960	0.6710
Q	0.8410	0.6790
R	0.7300	0.6200
S	0.6630	0.5980
b	0.1030	0.3900